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Standard X-ray Diffraction Powder Patterns

Section 11—Data for 70 Substances

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- Volume 2, page 30. In column 2, the density of PbO (red) should be 9.334 g/cm^3 .
- Volume 4, page 60. In the table column 4, the d-spacing 3.36 should be 2.36.
- Volume 6, page 60. In the table column 2, the d-spacing 2.75 should be 1.75.
- Volume 7, page 29. In the table, the NBS d-spacing 1.426 should be 1.406.

Monograph 25

Section 4, page 31. In the reference 4, the formula should be $\text{KC}_6\text{H}_4\text{COOH-COO}$.

Section 7, page 2 } In each section, the formula for L_p should be:

Section 8, page 3 }
 Section 9, page 3 }
 Section 10, page 3 }
$$L_p = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$$

Section 8, page 3. The formula for B should be:

$$B = 4 \left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^2 b^2 c^2} \right]^{\frac{1}{3}}$$

Section 9, page 115. The index entry for ammonium chlorosmate, $(\text{NH}_4)_2\text{OsCl}_6$, should be Sec. 1m, pg. 6.

Section 10, page 11. In the sample description, line 2, BrF_2 should be BaF_2 .

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22151. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

NBS Publication	Number	NBS Publication	Number
Circular 539, Volume 1.....	PB 178 902	Monograph 25, Section 1.....	PB 178 429
Volume 2.....	PB 178 903	Section 2.....	PB 178 430
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Section 11. --- Data for 70 Substances

by

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Standard x-ray diffraction patterns are presented for 70 substances. Fifty-two of these patterns represent experimental data and 18 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,³ the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 70 compounds (52 experimental and 18 calculated patterns), and is the twenty-first of the series of "Standard X-ray Diffraction Powder Patterns."⁴

^{1,2}Consultant and Research Associates, respectively, of the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards.

³Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, Pa. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

⁴See previous page for other published volumes.

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data, color. A microscopic inspection for phase purity was also made on the non-opaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, using oils standardized in sodium light, in the refractive index range 1.40 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with lines from the sample, silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of 2 θ were taken at positions about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction for each region was then applied to the measured value of 2 θ . We have reported all data as K α_1 peaks because the internal standard corrections for all regions were established in terms of the K α_1 wavelength.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the 2 θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2 θ Angles, CuK α_1 λ = 1.54056 Å		
hkl	W a = 3.16516 Å ±.00004	Ag a = 4.08641 Å ±.00002
110	40.262°	
111		38.112°
200	58.251	44.295
211	73.184	
220	86.996	64.437
310	100.632	
311		77.390
222	114.923	81.533
321	131.171	
400	153.535	97.875
331		110.499
420		114.914
422		134.871
511		156.737

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a curved lithium fluoride crystal monochromator located between the sample and the Geiger counter. Copper radiation was used and the wavelength K α_1 was taken to be 1.54056 Å [Bearden, 1964].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention $b > a > c$ [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary, in order to follow the convention of using a cell with the three shortest edges [Crystal Data, Vol. II, 1973].

A computer program [Evans et al. 1963] assigned hkl's and refined the lattice constants. Cell refinement was based only upon 2 θ_{obs} values which could be indexed without ambiguity. The program minimized the value $\sum (\theta_{\text{obs}} - \theta_{\text{calc}})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Beginning with this issue, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertain-

ty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. In indexing cubic patterns, multiple hkl's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the NBS determined lattice constants, the Avogadro number (6.02252×10^{23}), and atomic weights based on carbon 12 [International Union, 1961].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm , as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

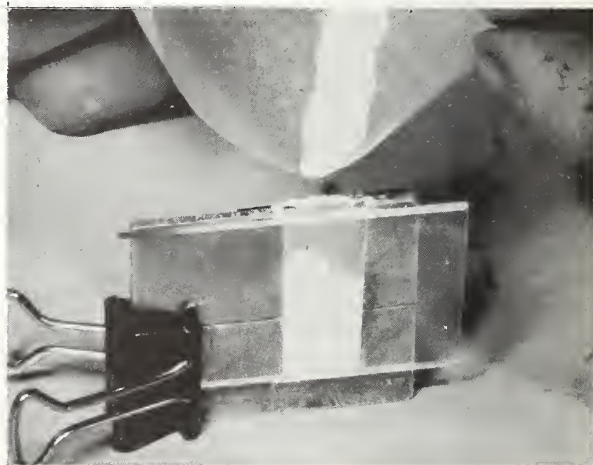


Figure 1

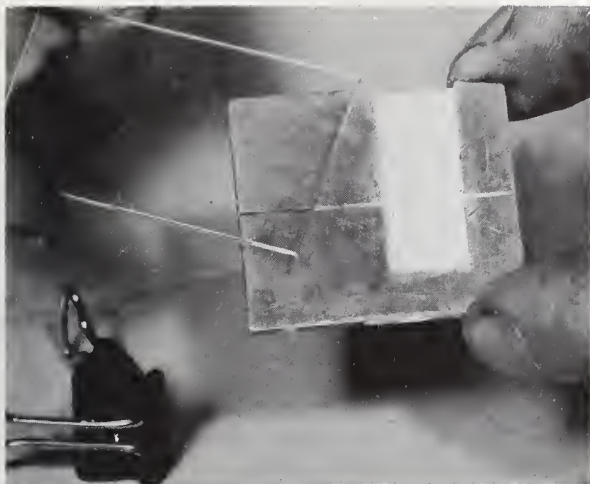


Figure 2

Reference intensity, I/I_{corundum} . For reference intensity measurements, $\alpha\text{-Al}_2\text{O}_3$ (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture of two components was mounted in our regular intensity sample holder (see Figures 1 and 2), and the pattern was taken. The reference intensity was then calculated as the direct ratio of the strongest line of the sample to the strongest line of corundum (hexagonal reflection (113)). In a few instances, the strongest line of one of the components coincided with a line of the other. In that case, the second strongest line was measured, and the value for the strongest line was then calculated.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Smith [1967] and modified at NBS.

Lattice parameters. Before the computations of the patterns, changes were made as necessary in the lattice constants in order to make then consistent with the revised value of the copper wavelength [Bearden, 1964]; specifically, a published lattice constant in Å was multiplied by 1.00004. Both the altered parameter and the original published value are given. Monoclinic and triclinic lattice constants were transformed if necessary, to follow the convention of using a cell with the 3 shortest edges [Crystal Data, Vol. II, 1973].

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the International Tables for X-ray Crystallography, Vol. III, [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's or the anisotropic β_{ij} 's in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})}$$

Other thermal parameters were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, in place of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4 \left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^2 b^2 c^2} \right]^{1/3}$$

Integrated intensities. Intensity calculations were based on the copper $K\alpha_1$ wavelength, 1.54056 Å, determined by Bearden [1964]. The integrated intensities were computed from formula (1):

$$(1) \quad I = F^2 (L_p) (\text{FAC})$$

where F is the standard structure factor

FAC is the powder multiplicity

$$L_p = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$$

The intensities were scaled to the strongest line which was assigned a value of 100. Reflections were not reported which had scaled intensities of 0.7 or less.

Scale factor. For each compound, this factor multiplied by the reported integrated intensities will reproduce the unscaled intensities which were derived using formula (1).

Peak intensities. The integrated intensities can be transformed to a Cauchy profile with an appropriate variable half-width designated to simulate a diffractometer tracing [Smith, 1967]. The value of the half-width was chosen as 0.075° at 40° (2θ , $\text{CuK}\alpha_1$). Then the intensities were summed for the overlapping peak profiles, and the resulting new peak intensities were scaled to the strongest peak height which was assigned a value of 100. Reflections were not reported which had scaled peak heights of 0.7 or less. Adjacent peaks with nearly equal 2θ values usually cannot be experimentally resolved; therefore one composite peak was calculated in such instances. The 2θ angle of this peak was assigned the hkl of the reflection having the greatest integrated intensity; a plus sign (+) was used to indicate additional hkl 's.

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Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$

Sample

The sample was prepared by heating a 2:1 mixture of $\alpha\text{Al}_2\text{O}_3$ and Bi_2O_3 at 1000 °C. This was followed by grinding and reheating.

Color

Pale yellow

Structure

Orthorhombic, Pbam (55), $Z=2$, isostructural with $\text{Bi}_2\text{Ga}_4\text{O}_9$. The structure was determined by Eckerlin and Liebertz [1965].

NBS lattice constants:

$a = 7.719(1)\text{Å}$

$b = 8.109(1)$

$c = 5.6919(8)$

Density

(calculated) 6.244 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 3.1$

Additional patterns

1. PDF card 23-1006 [Surnina and Litvin, 1970].

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Eckerlin, P. and Liebertz, J. (1965). *Naturwissenschaften* 52, 540.
Surnina, V.S. and Litvin, B.N. (1970). *Soviet Phys. Cryst. English Transl.* 15, 527.

Internal standard Ag, $a = 4.08641\text{ Å}$ $\text{CuK}\alpha_1$, $\lambda = 1.54056\text{ Å}$; temp. 25 °C			
$d\text{ (Å)}$	I	hkl	$2\theta(^{\circ})$
5.68	75	001	15.58
4.055	12	020	21.90
3.989	5	111	22.27
3.862	10	200	23.01
3.591	35	120	24.77
3.485	25	210	25.54
3.301	19	021	26.99
3.192	20	201	27.93
3.034	100	121	29.41
2.971	85	211	30.05

$d\text{ (Å)}$	I	hkl	$2\theta(^{\circ})$
2.846	30	002	31.41
2.795	12	220	32.00
2.551	15	130	35.15
2.537	14	112	35.35
2.510	3	221	35.75
2.453	9	310	36.60
2.328	16	022,131	38.65
2.290	14	202	39.31
2.252	11	311	40.01
2.230	12	122	40.42
2.204	35	212	40.91
2.028	1	321,040	44.64
1.994	1	222	45.44
1.961	12	140	46.26
1.930	3	400	47.05
1.908	2	041	47.61
1.898	10	132,003	47.88
1.878	7	410	48.44
1.864	15	330	48.83
1.857	16	312	49.02
1.854	25	141	49.10
1.827	1	401	49.87
1.795	3	240	50.82
1.783	16	411	51.18
1.771	17	331	51.55
1.743	3	420	52.46
1.726	1	322	53.00
1.719	2	023	53.25
1.703	2	203	53.77
1.677	14	123	54.69
1.666	13	213,421	55.07
1.652	5	042	55.60
1.615	7	142	56.98
1.597	5	402	57.66
1.567	9	412	58.87
1.559	25	332	59.21
1.528	1	151	60.54
1.5222	2	133	60.80
1.5004	2	313	61.78
1.4954	2	250	61.98
1.4655	1	511	63.42
1.4465	6	251	64.35
1.4233	5	004	65.53
1.3989	6	521	66.82
1.3865	3	152	67.50
1.3722	2	350	68.30
1.3638	5	143	68.78

Aluminum nitrate hydrate, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation of an aqueous solution of $\text{Al}(\text{NO}_3)_3$. The crystals were filtered out and washed with ethyl alcohol.

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.401$, $N_\beta = 1.514$, $N_\gamma = 1.525$;
 $2V \approx 25^\circ$.

Structure

Monoclinic, $P2_1/c$ (14), $Z=4$, isostructural with $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ [Kannan and Viswamitra, 1965].

NBS lattice constants:

$a = 13.847(8)\text{\AA}$

$b = 9.617(2)$

$c = 10.908(5)$

$\beta = 95.68(2)^\circ$

Density

(calculated) 1.724 g/cm^3

Reference intensity

I/I_{corundum} 0.5

Additional patterns

1. PDF card 1-435 [Hanawalt et al., 1938]
2. PDF card 12-472 [Aluminium Lab. Ltd., Kingston Canada].

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Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938)
Ind. Eng. Chem. Anal. Ed. 10, 457.

Kannan, K. K. and Viswamitra, M. A. (1965). Acta Cryst. 19, 151.

Internal standard W, $a = 3.16516 \text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{\AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
7.87	1	110	11.24
7.20	12	011	12.29
6.55	70	$\bar{1}11$	13.51
6.21	60	111	14.26
5.60	14	210	15.81
5.22	6	$\bar{1}02$	16.97
4.89	18	102	18.13
4.82	25	211, 020	18.41
4.729	4	012	18.75
4.595	4	$\bar{1}12, 300$	19.30

$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
4.539	15	120	19.54
4.487	45	202	19.77
4.362	3	112	20.34
4.231	2	$\bar{1}21$	20.98
4.143	10	310, 121	21.43
4.074	60	202	21.80
3.994	45	$\bar{3}11$	22.24
3.943	50	220	22.53
3.762	30	311	23.63
3.639	12	221	24.44
3.599	65	022	24.72
3.541	6	$\bar{1}22$	25.13
3.449	9	$\bar{3}12, 400$	25.81
3.426	12	122	25.99
3.387	6	013	26.29
3.278	16	$\bar{2}22$	27.18
3.244	35	410, $\bar{3}21$	27.47
3.219	19	113	27.69
3.123	20	130	28.56
3.112	20	321	28.66
3.074	12	031	29.02
3.049	20	$\bar{4}02$	29.27
3.017	100	131	29.58
2.982	45	131	29.93
2.907	35	230, $\bar{4}12$	30.73
2.878	7	$\bar{1}23$	31.05
2.854	5	$\bar{3}13$	31.32
2.835	4	231	31.53
2.788	3	402, 123	32.08
2.779	7	231	32.18
2.761	18	032	32.40
2.680	6	$\bar{1}32$	33.41
2.615	20	$\bar{2}04, 104, +$	34.26
2.609	30	$014, \bar{2}32, +$	34.34
2.590	50	331	34.60
2.538	16	$\bar{3}23$	35.33
2.522	35	331, 114, +	35.57
2.446	3	$\bar{3}04, 204$	36.71
2.422	2	$\bar{3}32$	37.09
2.399	6	033	37.45
2.393	4	520, $\bar{1}33$	37.56
2.369	40	$\bar{3}14, 140, +$	37.95
2.363	25	$\bar{1}24, 024, +$	38.05
2.348	30	041, 430	38.31
2.326	4	431	38.68
2.307	12	$\bar{4}23, 141$	39.01
2.301	14	$\bar{2}24, 600, +$	39.16
2.271	16	240	39.65
2.263	8	$\bar{4}31, \bar{5}22$	39.80
2.242	10	$\bar{4}04, \bar{5}13, +$	40.19
2.210	2	$\bar{4}32, 241$	40.79
2.184	16	$\bar{1}42, \bar{4}14, +$	41.30

Aluminum tungsten oxide, $\text{Al}_2(\text{WO}_4)_3$

Sample

The sample was prepared by adding NaWO_4 solution to one of AlCl_3 and heating the precipitate two hours at 800 °C and 15 minutes at 900 °C.

Color

Colorless

Structure

Orthorhombic, Pnca (60), $Z=2$, isostructural with other tungstates and molybdates of the smaller trivalent rare-earth elements such as $\text{Gd}_2(\text{WO}_4)_3$ [Craig and Stephenson, 1968].

NBS lattice constants:

$a = 9.139(2)\text{\AA}$
 $b = 12.596(2)$
 $c = 9.060(2)$

Density

(calculated) 2.539 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 2.3$

Additional patterns

1. PDF card 18-72 [Waring, 1965] (incorrectly called $2\text{Al}_2\text{O}_3 \cdot 5\text{WO}_3$)

References

Craig, D. C. and Stephenson, N. C. (1968). Acta Cryst. B24, 1250.
Waring, J. (1965). J. Am. Ceram. Soc. 48, 493.

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25 °C			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
6.30	11	020	14.04
5.73	13	111	15.46
4.53	11	002	19.59
4.50	6	121	19.73
4.296	35	210	20.66
4.059	40	102	21.88
3.877	50	211	22.92
3.867	45	112	22.98
3.810	100	031	23.33
3.697	16	220	24.05

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
3.676	7	022	24.19
3.519	25	131	25.29
3.422	50	221	26.02
3.219	15	202	27.69
3.147	12	040	28.34
3.115	4	212	28.63
3.090	6	230	28.87
2.933	19	013	30.45
2.926	10	231	30.53
2.865	13	222	31.19
2.828	6	141	31.61
2.816	9	311	31.75
2.624	7	321	34.14
2.610	16	123	34.33
2.593	7	240	34.56
2.555	2	232	35.10
2.528	7	302	35.48
2.493	8	241	36.00
2.488	9	142	36.07
2.480	7	312	36.19
2.471	6	213	36.32
2.429	5	051	36.98
2.380	5	331	37.76
2.368	19	133	37.97
2.346	3	322,151	38.34
2.340	4	223	38.45
2.285	2	400	39.40
2.265	3	004	39.77
2.252	7	242	40.01
2.206	11	250	40.87
2.182	17	411	41.35
2.166	6	114,332	41.67
2.161	5	233	41.77
2.142	10	251,152	42.15
2.132	5	024	42.35
2.114	5	313	42.73
2.100	13	060	43.03
2.076	1	124	43.56
2.030	3	323,204	44.61
2.004	9	214	45.21
1.984	3	252	45.70
1.972	9	342	45.99
1.959	2	431	46.30
1.941	6	422	46.77
1.935	5	053	46.92
1.907	6	260	47.66
1.8926	3	153	48.03
1.8650	13	162	48.79
1.8490	13	440	49.24
1.8385	9	044	49.54
1.8271	3	234	49.87
1.7987	2	314	50.73
1.7931	5	015	50.88
1.7833	5	352	51.18

Ammonium copper fluoride, NH_4CuF_3

Sample

The sample was prepared by the reaction of Cu and Br in methanol; the product was added to a saturated methanol solution of NH_4HF_2 . The precipitate was filtered, and washed with methanol and ether. The sample was somewhat hygroscopic.

Color

Greenish white

Structure

Tetragonal, $P4mm$ (99), $Z=2$, similar to KCuF_3 , distorted perovskite. Crockett and Haendler [1960] gave a larger cell related to ours as $a \approx a\sqrt{2}$ and $c \approx 2c$. We found no lines which required the larger cell.

NBS lattice constants:

$$a = 6.0828(4)\text{\AA}$$

$$c = 3.8915(4)$$

Density

(calculated) 3.196 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 2.4$$

Additional patterns

- PDF card 22-41 [Clavan, 1969, Pennwalt Corp. King of Prussia, Penna.]

References

Crockett, D.S. and Haendler, H.M. (1960). J. Am. Chem. Soc. 82, 4158.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
4.300	100	110	20.64
3.889	35	001	22.85
3.041	35	200	29.35
2.885	55	111	30.97
2.719	4	210	32.92
2.395	3	201	37.52
2.230	4	211	40.42
2.150	50	220	41.98
1.946	19	002	46.64
1.924	18	310	47.20
1.882	15	221	48.31
1.773	15	112	51.50
1.725	14	311	53.05
1.640	8	202	56.04
1.5478	2	321	59.69
1.5208	9	400	60.86
1.4753	3	410	62.95
1.4429	17	222	64.53
1.4336	5	330	65.00
1.4166	5	401	65.88
1.3681	9	312	68.53
1.3601	5	420	68.99
1.3453	4	331	69.86
1.2970	2	003	72.87
1.2419	4	113	76.67
1.1983	6	402	80.00
1.1930	5	203,510	80.43
1.1755	2	412	81.88
1.1542	5	332	83.73
1.1407	5	511	84.95
1.1146	4	422	87.43
1.1109	3	223	87.80
1.0756	4	313,440	91.47
1.0169	4	512	98.48

Ammonium formate, HCOONH_4

Sample

The sample was obtained from the K and K Laboratories, Inc., Jamaica, N.Y. The material was somewhat hygroscopic.

Color

Colorless

Structure

Monoclinic, Pc (7), $Z=2$. The structure was determined by Nahringsbauer [1968].

NBS lattice constants

$$a = 3.8202(5) \text{ \AA}$$

$$b = 4.6816(6)$$

$$c = 9.118(1)$$

$$\beta = 91.12(1)^\circ$$

Density

(calculated) 1.284 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.5$$

Additional patterns

1. PDF card 14-756 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938).

Ind. Eng. Chem. Anal. Ed. 10, 457.

Nahringsbauer, I. (1968). Acta Cryst. B24, 565.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
4.555	55	002	19.47
4.164	65	011	21.32
3.819	10	100	23.27
3.266	14	012	27.28
2.954	100	110, 102	30.23
2.898	5	102	30.83
2.826	30	111	31.63
2.802	6	111	31.91
2.550	9	013	35.17
2.500	10	112	35.89
2.466	9	112	36.41
2.340	8	020	38.43
2.279	13	004	39.51
2.267	11	021	39.73
2.137	2	113	42.26
2.105	1	113	42.92
2.083	4	022	43.41
2.049	7	014	44.16
1.996	1	120	45.39
1.974	4	104	45.93
1.955	1	121	46.42
1.945	2	121	46.66
1.941	1	104	46.76
1.9095	1	200	47.58
1.8546	4	023	49.08
1.8350	1	122	49.64
1.8192	2	114	50.10
1.7932	<1	114	50.88
1.7733	2	202	51.49
1.7685	2	210	51.64
1.7490	1	202	52.26
1.7419	1	211	52.49
1.7296	1	211	52.89
1.6990	2	015	53.92
1.6758	2	123	54.73
1.6598	2	123, 212	55.30
1.6335	<1	105, 024	56.27
1.5635	2	115	59.03
1.5406	2	213	60.00
1.5380	2	031	60.11
1.5193	1	006	60.93
1.5085	1	124	61.41
1.4938	<1	124	62.08
1.4801	<1	220	62.72
1.4767	1	032	62.88
1.4646	1	221	63.46
1.4574	1	221	63.81
1.4451	1	016, 130	64.42
1.4283	2	131	65.27
1.4246	2	131	65.46

Ammonium lead chloride, $(\text{NH}_4)_2\text{PbCl}_6$

Sample

Chlorine was bubbled through a saturated solution of PbCl_2 in concentrated HCl . Then a saturated solution of NH_4Cl in concentrated HCl was added. The precipitate formed was filtered without washing.

Color

Brilliant green yellow

Structure

Cubic, $\text{Fm}3\text{m}$ (225), $Z=4$, isostructural with K_2PtCl_6 . The structure was determined by Wyckoff and Dennis [1926].

NBS lattice constant: $a = 10.1609(3)\text{\AA}$

Density

(calculated) 2.887 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 3.6$

Additional patterns

1. PDF card 2-0139 [Wyckoff and Dennis, 1926].

Reference

Wyckoff, R. W. G. and Dennis, L. M. (1926). Am. J. Sci. 12, 503.

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. $25\text{ }^\circ\text{C}$			
$d\text{ (\AA)}$	I	hkl	$2\theta(^\circ)$
5.866	100	111	15.09
5.081	45	200	17.44
3.593	20	220	24.76
3.061	45	311	29.15
2.933	1	222	30.45
2.540	25	400	35.31
2.332	18	331	38.57
2.272	25	420	39.63
2.074	9	422	43.61
1.955	14	511	46.41
1.796	15	440	50.78
1.718	12	531	53.29
1.693	10	600	54.11
1.607	2	620	57.28
1.5495	4	533	59.62
1.4667	3	444	63.36
1.4229	4	711	65.55
1.4090	2	640	66.28
1.3577	2	642	69.13
1.3227	4	731	71.23
1.2701	<1	800	74.67
1.2415	1	733	76.70
1.2324	3	820	77.37
1.1976	1	822	80.06
1.1733	2	751	82.07
1.1359	2	840	85.39
1.1152	2	911	87.37
1.1087	2	842	88.02
1.0829	<1	664	90.68
1.0652	1	931	92.63
1.0369	1	844	95.95
1.0211	2	933	97.94
1.0161	1	10·0·0	98.59
0.9964	1	10·2·0	101.25
0.9823	1	951	103.28

Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution containing 2 grams NH_4Cl and 3.6 grams $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$. The first crystals formed were used. The method follows the phase study of the $\text{NH}_4\text{Cl}-\text{MnCl}_2-\text{H}_2\text{O}$ system by Clendinnen and Rivett [1921].

Color

Pinkish white

Structure

Tetragonal, $P4_2/mnm$ (136), $Z=2$, isostructural with $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ [Greenberg and Walden, 1940]. The structure of $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ was determined by Hendricks and Dickerson [1927] and refined by Chrobak, [1934]. Greenberg and Walden [1940] found $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ to have a solid solution relation with $(\text{NH}_4)_6\text{MnCl}_8 \cdot 2\text{H}_2\text{O}$.

NBS lattice constants:

$a = 7.589(1) \text{ \AA}$

$c = 8.143(2)$

Density

(calculated) 1.904 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 1.4$

References

- Chrobak, L. (1934). Z. Krist. **88**, 35.
Clendinnen, F.W.J. and Rivett, A.C.D. (1921). J. Chem. Soc. **119**, 1329.
Greenberg, A.L. and Walden, G. H. Jr. (1940). J. Chem. Phys. **8**, 645.
Hendricks, S.B. and Dickerson, R.G. (1927). J. Am. Chem. Soc. **49**, 2149.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
5.552	35	101	15.95
5.365	15	110	16.51
4.073	35	002	21.80
3.797	6	200	23.41
3.244	8	112	27.47
3.131	8	211	28.48
2.776	100	202	32.22
2.684	90	220	33.36
2.557	8	103	35.06
2.401	4	310	37.43
2.240	25	222	40.22
2.120	5	213	42.61
2.067	1	312	43.76
2.038	19	321	44.41
1.898	16	400	47.89
1.798	3	313	50.72
1.7938	5	204	50.86
1.7194	8	402	53.23
1.6629	4	323	55.19
1.6213	17	224	56.73
1.5660	9	422	58.93
1.5231	2	413	60.76
1.4923	2	431	62.15
1.3877	8	521,404	67.43

Additional patterns

1. PDF card 2-844 [Greenberg and Walden, 1940].

Barium hydroxide phosphate, $\text{Ba}_5(\text{OH})(\text{PO}_4)_3$

Sample

The sample was prepared by heating $\text{Ba}(\text{OH})_2$ and $(\text{NH}_4)_2\text{HPO}_4$ together in a molar ratio of 5 : 3. After heating at 300 °C, the material was pelletized and reheated at 600 °C for one hour, at 900 °C for one hour, and at 1100 °C for one half hour.

Color

Colorless

Structure

Hexagonal, $P6_3/m$ (176), $Z=2$, isostructural with calcium and lead hydroxyapatites [Klement and Dihn, 1938]. The structure of $\text{Ca}_5(\text{OH})(\text{PO}_4)_3$ was refined by Posner et al. [1958].

NBS lattice constants:
 $a = 10.185(1)\text{\AA}$
 $c = 7.729(1)$

Density

(calculated) 4.728 g/cm³

Reference intensity

$I/I_{\text{corundum}} = 2.5$

Additional patterns

1. PDF card 1-811 [Hanawalt et al., 1938]
2. PDF card 3-578 [Klement and Dihn, 1938]

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Klement, R. and Dihn, P. (1938). Z. anorg. u. allgem. Chem. 240, 40.
 Posner, A.S., Perloff, A., and Diorio, A.F. (1958). Acta Cryst. 11, 308.

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25 °C			
$d\text{ (\AA)}$	I	hkl	$2\theta\text{ (}^\circ\text{)}$
5.10	3	110	17.37
4.410	25	200	20.12
4.255	19	111	20.86
3.869	12	002	22.97
3.829	1	201	23.21
3.541	30	102	25.13
3.334	35	210	26.72
3.079	100	112	28.98
3.062	100	211	29.14
2.940	50	300	30.38
2.908	4	202	30.72
2.546	2	220	35.22
2.447	8	310	36.70
2.338	5	302	38.47
2.334	2	311	38.54
2.299	11	113	39.15
2.225	2	203	40.50
2.205	3	400	40.90
2.127	30	222	42.47
2.067	25	312	43.76
2.038	30	213	44.41
2.023	6	320	44.77
1.958	17	321	46.34
1.932	12	004	47.00
1.925	20	410	47.18
1.915	25	402	47.43
1.868	1	411	48.70
1.807	1	114	50.45
1.792	<1	322	50.91
1.775	1	313	51.45
1.769	3	204	51.62
1.7230	3	412	53.11
1.6979	<1	330	53.96
1.6721	10	214	54.86
1.6671	8	420	55.04
1.6582	3	331	55.36
1.6290	1	421	56.44
1.6143	8	304	57.00
1.6048	5	502	57.37
1.5913	8	323	57.90

Barium lead chloride, BaPbCl₄

Sample

The sample was prepared by melting an equimolar mixture of BaCl₂ and PbCl₂. It was then ground and heated for 18 hours, at 400 °C, in a sealed glass tube. This was repeated twice.

Color

Colorless

Structure

Orthorhombic, Pnam (62), $Z = 2$; BaCl₂ and PbCl₂ form a complete solid solution series [Calingaert et al., 1949]. The structure of BaCl₂ was determined by Döll and Klemm [1939] and refined by Brackett et al. [1963] and Sahl [1963].

NBS lattice constant:

$a = 7.765(2) \text{ \AA}$
 $b = 9.246(2)$
 $c = 4.658(1)$

Density

(calculated) 4.829 g/cm³

Reference intensity

$I/I_{\text{corundum}} = 2.8$

References

- Brackett, E. B., Brackett, T. E., and Sass, R. L. (1963). J. Phys. Chem. 67, 2132.
 Calingaert, G., Lamb, F. W., and Meyer, F. (1949). J. Am. Chem. Soc. 71, 3712.
 Döll, W. and Klemm, W. (1939). Z. anorg. u. allgem. Chem. 241, 239.
 Sahl, K. (1963). Beitr. Mineral. Petrog. 9, 111.

Internal standard W, $a = 3.16516 \text{ \AA}$ CuK α_1 $\lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d \text{ (\AA)}$	I	hkl	$2\theta \text{ (}^\circ\text{)}$
4.62	11	020	19.20
4.16	40	011	21.35
3.97	95	120	22.40
3.885	55	200	22.87
3.664	100	111	24.27
3.020	13	121	29.55
2.981	14	201	29.95
2.972	20	220	30.04
2.866	11	130	31.18
2.838	80	211	31.50
2.572	50	031	34.86
2.508	4	221	35.77
2.440	12	131	36.80
2.415	5	230	37.20
2.331	30	002	38.60
2.311	19	040	38.94
2.259	35	320	39.87
2.215	7	140	40.70
2.197	35	311	41.05
2.142	40	231	42.15
2.081	2	022	43.45
2.009	20	122	45.08
1.997	17	202	45.38
1.986	11	240	45.63
1.941	7	400	46.76
1.833	3	222	49.71
1.759	2	411	51.94
1.678	10	151	54.64
1.675	7	232	54.76
1.642	7	430	55.96
1.6216	15	322	56.72
1.6053	3	142	57.35
1.5720	<1	251	58.68
1.5492	4	431	59.63
1.5110	6	242	61.30
1.5023	5	113	61.69
1.4910	5	402	62.21
1.4869	5	440	62.40
1.4556	7	511	63.90
1.4318	8	351	65.09

Barium nitrate (nitrobarite), Ba(NO₃)₂ (revised)

Sample

The sample was specially purified material from Mallinckrodt Chemical Works, New York.

Major impurities

0.001–0.01% each: Al, Na, and Sr.

Color

Colorless

Optical data

Isotropic, $n = 1.571$

Structure

Cubic, $P2_13$ (198), $Z = 4$, isostructural with Sr(NO₃)₂. The structure was determined by Birnstock [1967]. Previously the space group of Ba(NO₃)₂ was considered to be $Pa\bar{3}$ (205).

NBS lattice constant:
 $a = 8.1184(2)\text{\AA}$

Density

(calculated) 3.244 g/cm³

Reference intensity

$I/I_{\text{corundum}} = 4.5$

Additional patterns

1. PDF card 4-773 [Swanson and Tatge, 1953]

Internal standard W, $a = 3.16516\text{\AA}$ CuK α_1 $\lambda = 1.54056\text{\AA}$; temp. 25 °C			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
4.689	100	111	18.91
4.062	35	200	21.86
3.633	14	210	24.48
3.318	10	211	26.85
2.870	30	220	31.14
2.447	75	311	36.69
2.344	45	222	38.37
2.170	<1	321	41.59
2.031	12	400	44.58
1.970	<1	410	46.04

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
1.914	1	330	47.46
1.863	20	331	48.85
1.816	17	420	50.19
1.772	1	421	51.53
1.732	1	332	52.82
1.658	13	422	55.37
1.5923	<1	510	57.86
1.5626	11	333	59.07
1.5079	1	432	61.44
1.4827	<1	521	62.60
1.4352	8	440	64.92
1.3919	1	530	67.20
1.3723	15	531	68.29
1.3532	7	600	69.39
1.3348	1	610	70.49
1.3171	1	611	71.58
1.2836	3	620	73.75
1.2681	<1	621	74.81
1.2380	5	533	76.95
1.2237	5	622	78.02
1.2103	<1	630	79.05
1.1719	2	444	82.19
1.1367	5	551	85.32
1.1259	2	640	86.34
1.1151	1	720	87.38
1.0848	4	642	90.48
1.0570	5	731	93.56
1.0149	<1	800	98.75
1.0071	<1	740	99.79
.9918	1	733	101.91
.9844	2	820	102.98
.9567	2	660	107.24
.9375	3	751	110.50
.9313	1	662	111.61
.9078	1	840	116.11
.8910	2	911	119.65
.8857	1	842	120.84
.8654	1	664	125.76
.8510	1	931	129.69
.8285	1	844	136.80
.8158	2	755	141.53
.8119	1	860	143.17
.7960	2	10·2·0	150.78
.7848	<1	951	157.94

References

Birnstock, R. (1967). Z. Krist. 124, 310.
Swanson, H.E. and Tatge, E. (1953). Natl. Bur. Std. U.S. Circ. 539, 1, 81.

Cadmium bromide chloride, CdBrCl

Sample

The sample was prepared by melting a 1:1 molar mixture of CdBr₂ and CdCl₂. This was then annealed for three days at 300°C in a sealed tube.

Color

Light grey

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$, isostructural with CdCl₂. The structure of CdCl₂ was determined by Pauling [1929]. A complete solid solution exists between CdBr₂ and CdCl₂ [Nacken, 1907].

NBS lattice constants:

$$a = 3.9204(3) \text{ \AA}$$

$$c = 18.408(2)$$

Density

(calculated) 4.630 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 3.3$$

References

- Nacken, R. (1907). Centr. Mineral Geol. 1907, 303.
Pauling, L. (1929). Proc. Nat. Acad. Sci. U.S. 15, 709.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d \text{ (\AA)}$	I	hkl	$2\theta \text{ (}^\circ\text{)}$
6.137	100	003	14.42
3.340	30	101	26.67
3.068	1	006	29.08
2.734	60	104	32.73
2.496	10	015	35.95
2.081	6	107	43.46
2.046	3	009	44.23
1.961	25	110	46.26
1.905	17	018	47.70
1.868	10	113	48.71
1.690	3	021	54.22
1.5928	7	024	57.84
1.5417	1	205	59.95
1.5338	4	0.0.12	60.29
1.5013	1	0.1.11	61.74
1.4268	1	027	65.35
1.4154	2	119	65.94
1.3662	3	208	68.64
1.3070	<1	1.0.13	72.22
1.2801	2	211	73.99
1.2359	4	214	77.11
1.2272	1	0.0.15	77.76
1.2116	1	125	78.95
1.2079	4	1.1.12	79.24
1.1917	<1	2.0.11	80.53
1.1534	1	217	83.80
1.1317	2	300	85.79
1.1206	2	128	86.85
1.1129	<1	303	87.60
1.0897	1	1.0.16	89.96
1.0400	<1	1.1.15	95.57
1.0315	<1	0.1.17	96.62
1.0183	<1	1.2.11	98.30

Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$

Sample

The sample was prepared by treating a saturated solution of CaO with 6 % phenol. Aluminum metal dissolved in KOH was added. The compound was then dried at 110°C for two hours.

Color

Colorless

Optical data

Isotropic, $N = 1.605$

Structure

Cubic, $\text{Ia}\bar{3}\text{d}$ (230), $Z = 8$, garnet type [Flint et al., 1941].

NBS lattice constant:
 $a = 12.5727(2)\text{\AA}$

Density

(calculated) 2.527 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 1.0$

Additional patterns

1. PDF 3-125 [Flint et al., 1941]

References

Flint, E.P., McMurdie, H.F., and Wells, L.S. (1941)
J. Res. Natl. Bur. Std. 26, 13.

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1\ \lambda = 1.54056\text{\AA}$; temp. 25°C			
$d\ (\text{\AA})$	I	hkl	$2\theta(^{\circ})$
5.130	90	211	17.27
4.442	40	220	19.97
3.358	55	321	26.52
3.142	45	400	28.38
2.810	80	420	31.82
2.680	6	332	33.41
2.566	15	422	34.94
2.465	30	431	36.42
2.295	100	521	39.23
2.222	4	440	40.56
2.039	95	611	44.39
1.989	8	620	45.58
1.8536	1	631	49.11
1.8148	10	444	50.23
1.7785	2	543	51.33
1.7437	40	640	52.43
1.7111	20	721	53.51
1.6800	50	642	54.58
1.5964	11	732	57.70
1.5715	13	800	58.70
1.5478	1	741	59.69
1.5249	1	820	60.68
1.5030	2	653	61.66
1.4818	3	660	62.64
1.4616	1	831	63.61
1.4243	1	752	65.48
1.4058	12	840	66.45
1.3716	5	842	68.33
1.3555	5	761	69.26
1.3401	8	664	70.17
1.3253	2	851	71.07
1.2965	5	932	72.90
1.2835	2	844	73.76
1.2701	4	941	74.67
1.2449	2	10·1·1	76.45
1.2330	1	10·2·0	77.32
1.2216	1	943	78.18
1.1986	8	10·3·1	79.98
1.1774	<1	871	81.72
1.1673	8	10·4·0	82.58
1.1574	4	10·3·3	83.45
1.1478	10	10·4·2	84.30
1.1382	1	873	85.18
1.1202	8	11·2·1	86.89
1.1113	4	880	87.76

Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$ – continued

d (Å)	I	hkl	2θ (°)
1.0863	4	11·3·2	90.32
1.0624	1	10·6·2	92.94
1.0551	2	965	93.78
1.0478	2	12·0·0	94.64
1.0406	1	11·4·3	95.50
1.0337	2	12·2·0	96.35
1.0266	2	11·5·2	97.24
1.0197	5	12·2·2	98.12
1.0132	1	12·3·1	98.97
0.9758	5	11·6·3	104.26
.9532	2	13·2·1	107.83
.9477	1	12·4·4	108.74
.9371	5	12·6·0	110.56
.9320	3	13·3·2	111.47
.9268	3	12·6·2	112.43
.9220	1	13·4·1	113.33
.9073	1	888	116.19
.8935	1	13·5·2	119.11
.8890	1	14·2·0	120.09
.8846	1	12·7·3	121.10
.8760	3	14·3·1	123.13
.8718	2	12·8·0	124.15
.8675	<1	13·5·4	125.23
.8635	3	14·4·0	126.26
.8593	<1	14·3·3	127.38
.8554	8	14·4·2	128.44

Calcium chloride (hydrophilite), CaCl_2

Sample

CaCO_3 was slowly converted to CaCl_2 by exposure to dry HCl fumes. However, since a few peaks of another phase persisted in the sample it was felt that intensity values should be calculated rather than measured.

Color

Colorless

Structure

Orthorhombic, Pnmm (58), $Z=2$, distorted rutile arrangement. The structure was determined by van Bever and Nieuwenkamp [1935]. Intensity values were calculated from structure data using the following information:

NBS lattice constants:

$a = 6.261(2)\text{\AA}$

$b = 6.429(2)$

$c = 4.167(1)$

Atom positions:

Ca (0 0 0)

Cl (.275 .325 0) [van Bever and Nieuwenkamp, 1935]

Scattering factors:

Ca^{2+} , Cl^- [International Tables, 1962]

Thermal parameters:

overall $B = 1.0$

Density

(calculated) 2.175 g/cm^3

Polymorphism

Jensen [1943] described 3 modifications.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I (calc.)	hkl	$2\theta (^\circ)$
4.48	85	110	19.80
3.46	17	101	25.71
3.050	100	111	29.26
2.858	35	120	31.27
2.816	4	210	31.75
2.356	25	121	38.16
2.331	50	211	38.59
2.244	30	220	40.16
2.083	20	002	43.40
2.027	3	130	44.66
1.974	2	221	45.94
1.906	25	031	47.68
1.890	10	112	48.10
1.866	11	301	48.75
1.792	10	311	50.92
1.751	4	320	52.20
1.684	7	122	54.44
1.565	4	400	58.97
1.527	10	222	60.59
1.496	4	330	62.00

Additional patterns

1. PDF card 1-0338 [Hanawalt et al., 1938]
2. Döll and Klemm [1939]

References

- van Bever, A. K. and Nieuwenkamp, W. (1935). *Z. Krist.* **90**, 374.
- Döll, W. and Klemm, W. (1939). *Z. anorg. u. allgem. Chem.* **241**, 233.
- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938) *Ind. Eng. Chem. Anal. Ed.* **10**, 457.
- International Tables **III** (1962). 202, 204.
- Jensen, A.T. (1943). *Kgl. Danske Videnskab. Selskab* **20** #5, 1.

Cesium cobalt chloride, Cs_2CoCl_4

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 aqueous solution of CsCl and CoCl_2 .

Color

Brilliant greenish blue

Optical data

Biaxial, $N_\alpha = 1.575$, $N_\beta = 1.585$, $N_\gamma = 1.596$; $2V$ is very large.

Structure

Orthorhombic, Pnam (62), $Z=4$, isostructural with K_2SO_4 and Cs_2CuCl_4 [Porai-Koshitz, 1954]. The structure was determined by Tishchenko and Pinsker [1955].

NBS lattice constants:

$$a = 9.771(2) \text{ \AA}$$

$$b = 12.973(2)$$

$$c = 7.401(1)$$

Density

(calculated) 3.303 g/cm^3

Reference intensity

I/I_{corundum} 1.8

Major impurities

~ .05% Al, Cu, Si, and Zn.

References

Porai-Koshitz, M.A. (1954). Tr. Inst. Kristallogr. Akad. Nauk SSSR **10**, 269.

Tishchenko, G.N. and Pinsker, Z.G. (1955). Dokl. Akad. Nauk SSSR **100**, 913.

Internal standard Ag , $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1$, $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
4.569	18	210	19.41
4.367	90	121	20.32
4.075	15	201	21.79
3.952	19	130	22.48
3.889	75	211	22.85
3.731	95	031	23.83
3.697	100	002	24.05
3.485	10	131	25.54
3.454	10	221	25.77
3.345	4	112	26.63
3.242	70	040	27.49
3.157	75	310	28.24
3.075	14	140	29.01
3.053	35	122	29.23
2.947	11	202	30.30

$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
2.904	40	311	30.76
2.875	55	212	31.08
2.841	30	141	31.46
2.700	35	240,132	33.15
2.684	30	222	33.36
2.600	40	330	34.46
2.537	8	241	35.35
2.507	12	150	35.78
2.447	20	051	36.70
2.436	40	232	36.87
2.402	20	312,410	37.41
2.319	5	401	38.80
2.297	8	340	39.18
2.284	16	411	39.42
2.245	13	123	40.14
2.194	19	341	41.11
2.170	10	213	41.59
2.142	13	033	42.16
2.126	9	332,430	42.48
2.093	2	133	43.18
2.086	4	223	43.35
2.076	11	152	43.57
1.976	6	260	45.88
1.951	11	342,440	46.50
1.945	13	422,313	46.66
1.925	6	143	47.17
1.910	5	261	47.56
1.870	13	520,511	48.65
1.850	16	004	49.21
1.843	13	432	49.40
1.822	3	243,170	50.03
1.798	10	071	50.74
1.779	5	352,024 +	51.30
1.750	5	124,361	52.24
1.744	14	262	52.41
1.730	6	531,204	52.88
1.714	7	512	53.42
1.687	3	271	54.32
1.682	8	343	54.50
1.670	18	522	54.93
1.632	9	541	56.31
1.629	8	600	56.45
1.622	3	080	56.69
1.6068	11	044	57.29
1.6037	9	163,452	57.41
1.6004	10	180	57.54
1.5969	9	314	57.68
1.5911	7	601	57.91
1.5858	4	144	58.12
1.5431	2	263	59.89
1.5276	7	551	60.56
1.5081	6	334	61.43
1.4891	5	154	62.30

Cesium copper chloride, Cs_2CuCl_4

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 molar aqueous solution of CsCl and CuCl_2 .

Color

Unground - deep brown
Ground - deep orange

Optical data

Biaxial (+), $N_\alpha = 1.625$, $N_\beta = 1.648$, $N_\gamma = 1.678$
 $2V = 83^\circ 46'$ [Helmholz and Kruh, 1952].

Structure

Orthorhombic, Pnm (62), $Z = 4$. The space group was determined by Mellor [1939]. The structure was determined by Helmholz and Kruh [1952], and refined by Morosin and Lingafelter [1961].

NBS lattice constants:
 $a = 9.773(2)\text{\AA}$
 $b = 12.415(2)$
 $c = 7.617(2)$

Density

(calculated) 3.386 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 1.2$

References

- Helmholz, L. and Kruh, R.F. (1952). J. Am. Chem. Soc. 74, 1176.
Mellor, D.P. (1939). Z. Krist. 101A, 160.
Morosin, B. and Lingafelter, E.C. (1961). J. Phys. Chem. 65, 50.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.236	2	120	16.92
4.546	11	210	19.51
4.316	55	121	20.56
4.116	25	201	21.57
3.905	40	211	22.75
3.841	35	220	23.14
3.808	100	130,002	23.34
3.638	50	031	24.45
3.410	5	112,131	26.11
3.247	2	022	27.45
3.157	60	230	28.24
3.152	60	310	28.29
3.103	60	040	28.75
3.082	30	122	28.95
3.005	16	202	29.71
2.959	4	140	30.18
2.920	25	212,231	30.59
2.913	25	311	30.67
2.884	25	320	30.98
2.758	16	141	32.43
2.704	25	222	33.10
2.696	25	321,132	33.20
2.560	30	330	35.02
2.477	12	241	36.23
2.442	9	400	36.77
2.429	35	232,312	36.97
2.406	25	150,042	37.35
2.361	3	051	38.09
2.300	7	322	39.14
2.286	20	411,123	39.38
2.274	6	420	39.60
2.253	5	203	39.99
2.247	3	340	40.09
2.217	12	213	40.67
2.179	2	421	41.40
2.164	11	033	41.71
2.156	13	242,341	41.87
2.124	10	251,332	42.53
2.056	2	402	44.00
2.033	11	152	44.52
2.028	10	412,431	44.64
1.980	5	233	45.79
1.977	3	313,350	45.86
1.953	3	422	46.47
1.935	5	342	46.92
1.929	7	510,143	47.06
1.910	8	351	47.56
1.904	25	260,004	47.72
1.872	5	511	48.60
1.864	7	520	48.82

Cesium copper chloride, Cs_2CuCl_4 – continued

d (Å)	I	hkl	2θ (°)
1.848	2	261,114	49.26
1.842	4	432	49.45
1.823	3	243	49.99
1.819	4	062	50.12
1.788	4	124,162	51.04
1.7673	3	530	51.68
1.7562	2	214	52.03
1.7428	5	413	52.46
1.7269	14	071	52.98
1.7218	16	512,531	53.15
1.7031	17	262,134	53.78
1.6979	11	451	53.96
1.6826	4	343	54.49
1.6746	6	522	54.77
1.6668	4	270	55.05
1.6546	3	540	55.49
1.6298	12	314,600	56.41
1.6234	8	044	56.65
1.6169	9	541	56.90
1.6030	9	532	57.44
1.5886	6	324	58.01
1.5786	6	611,460	58.41
1.5590	3	353	59.22
1.5366	3	513,550	60.17
1.5276	9	334,272	60.56
1.5166	5	542	61.05

Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by evaporating an aqueous solution of CoCl_2 at about 90 °C. The first crystals formed were filtered from the solution and washed with ethyl alcohol. The sample forms a higher hydrate in moist air.

Color

Deep violet

Structure

Monoclinic, C2/m (12), $Z = 2$, isostructural with $\text{CoBr}_2 \cdot 2\text{H}_2\text{O}$ and the corresponding Mn salts [Morosin, 1965]. The structure of $\text{CoBr}_2 \cdot 2\text{H}_2\text{O}$ was determined by Morosin and Graeber [1963].

NBS lattice constants:

$a = 7.280(1)\text{\AA}$

$b = 8.552(2)$

$c = 3.573(1)$

$\beta = 97.55(1)^\circ$

Density

(calculated) 2.498 g/cm^3

Reference intensity

$I/I_0 = 2.5$

Additional patterns

1. PDF card 3-786 [Neuhaus, 1938].

References

- Morosin, B. (1965). Abstract Bull. Am. Phys. Soc. 10, 686.
Morosin, B. and Graeber, E.J. (1963). Acta Cryst. 16, 1176.
Neuhaus, A. (1938). Z. Krist. 98, 112.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
5.514	100	110	16.06
4.277	65	020	20.75
3.606	2	200	24.67
3.542	3	001	25.13
3.127	4	$\bar{1}11$	28.52
2.854	25	111	31.32
2.758	14	220	32.43
2.726	20	021	32.83
2.712	40	201	33.00
2.651	11	130	33.78
2.376	25	201	37.84
2.315	4	310	38.87
2.291	12	$\bar{2}21$	39.30
2.138	20	040	42.23
2.076	19	131, 221	43.56
2.0611	12	$\bar{3}11$	43.89
1.8350	4	311	49.64
1.8044	8	400	50.54
1.7711	6	002	51.56
1.7379	6	$\bar{1}12$	52.62
1.7031	5	$\bar{3}31$	53.78
1.6789	10	$\bar{2}41$	54.62
1.6626	6	420	55.20
1.6359	3	022	56.18
1.5896	10	241	57.97
1.4233	3	510	65.53
1.3938	1	350	67.09
1.3786	5	440	67.94

Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of CoCl_2 .

Color

Deep purplish red

Optical data

Biaxial (+), $N_\alpha=1.524$, $N_\beta=1.548$, $N_\gamma=1.580$. 2V is very large.

Structure

Monoclinic, $I2/m$ (12), $Z = 2$, isostructural with $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$. The structure was determined by Mizuno (1960).

NBS lattice constants:

$a = 8.898(2) \text{ \AA}$

$b = 7.066(1)$

$c = 6.644(1)$

$\beta = 97.25(1)^\circ$

Density

(calculated) 1.907 g/cm^3

Polymorphism

1. PDF card 13-399 [Inst. of Physics, University College, Cardiff, Wales] reports a cell related to this form but with the c doubled and with space group $P2_1/c$ (14). The pattern however appears quite different, so a polymorph may exist.

References

Mizuno, J. (1960). J. Phys. Soc. Japan **15**, 1412.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.636	100	$\bar{1}01$	15.71
5.521	45	110	16.04
4.987	15	101	17.77
4.826	55	011	18.37
4.421	4	200	20.07
3.534	18	020	25.18
3.414	4	$\bar{2}11$	26.08
3.115	11	211	28.63
2.993	16	$\bar{1}21$	29.83
2.933	55	$\bar{1}12$	30.45
2.817	20	$\bar{2}02$	31.74
2.758	30	220	32.44
2.735	16	112	32.72
2.716	35	310	32.95
2.569	19	301	34.89
2.410	30	022	37.28
2.219	10	031	40.63
2.206	25	400, $\bar{3}21$	40.87
2.079	10	$\bar{4}11$, $\bar{3}21$	43.49
2.038	7	222	44.41
1.985	18	312	45.66
1.951	5	$\bar{4}02$, $\bar{2}31$	46.51
1.940	5	411	46.80
1.902	17	$\bar{1}32$	47.77
1.871	8	420	48.62
1.8664	8	$\bar{1}23$	48.75
1.8388	4	330	49.53
1.8118	4	213	50.32
1.7873	3	123	51.06
1.7666	7	040	51.70
1.7075	15	$\bar{4}22$	53.63
1.6852	3	$\bar{1}41$	54.40
1.6136	9	$\bar{1}14$	57.03
1.6115	8	$\bar{2}04$	57.11
1.5989	6	431	57.60
1.5769	3	$\bar{5}21$	58.48
1.5564	10	042, $\bar{2}33$	59.33
1.5540	6	332	59.43
1.5041	4	323	61.61
1.4932	3	024	62.11
1.4837	3	204	62.55
1.4694	5	$\bar{5}03$	63.23
1.4665	5	233, $\bar{2}24$	63.37
1.4554	3	341	63.91

Cobalt fluoride hydrate, $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation of an aqueous solution of CoF_2 at room temperature.

Color

Medium red

Structure

Orthorhombic, $\text{P2}_1\text{ab}$ (29), $Z = 4$, isostructural with $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ and other similar tetrahydrates. The structure of $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ was investigated by Rao et al. [1965].

NBS lattice constants:

$$\begin{aligned} a &= 7.552(2) \text{ \AA} \\ b &= 12.658(3) \\ c &= 5.287(1) \end{aligned}$$

Density

(calculated) 2.221 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.8$$

Polymorphism

Easwaran and Srinivasan [1965] reported, by comparison of powder patterns, that $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ was isostructural with $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$. However, Penfold and Taylor [1960] reported $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ as rhombohedral. This suggests a second form of $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ exists.

Additional patterns

1. PDF card 1-258 [Hanawalt et al., 1938]

References

- Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.
Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. 13, 953.
Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. 3, 68.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.289	5	001	16.75
4.854	100	120, 011	18.26
4.096	35	111	21.68
3.776	4	200	23.54
3.577	3	121	24.87
3.296	4	031	27.03
3.165	25	040	28.17
3.071	3	201	29.05
3.019	5	131	29.56
2.987	30	211	29.89
2.919	2	140	30.60
2.764	15	221	32.36
2.644	1	002	33.88
2.589	3	012	34.62
2.557	7	141	35.07
2.484	3	231	36.13
2.448	5	112	36.68
2.338	3	320	38.48
2.321	4	122	38.76
2.281	2	051	39.47
2.237	7	311	40.29
2.186	8	151	41.26
2.165	14	202	41.68
2.136	4	212	42.28
2.031	20	160	44.58
2.001	4	331	45.28
1.959	6	061, 142	46.31
1.954	7	251	46.44
1.927	3	232	47.12
1.889	6	400	48.14
1.845	1	341	49.34
1.8044	5	312	50.54
1.7869	8	242	51.07
1.7606	5	411	51.89
1.7515	11	322	52.18
1.7465	7	013	52.34
1.7117	2	421, 071	53.49
1.6921	2	351	54.16
1.6732	3	332	54.82
1.6696	3	171	54.95
1.6563	3	123	55.43
1.6456	3	252	55.82
1.6213	3	440	56.73
1.6169	3	360	56.90
1.5893	2	133	57.98

Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation of a CuF_2 aqueous solution at room temperature.

Color

Brilliant greenish blue

Optical data

Biaxial (-), $N_\alpha = 1.502$, $N_\beta = 1.522$, $N_\gamma = 1.534$; 2V is medium large.

Structure

Monoclinic, $I2/m$ (12), $Z=2$. The structure was determined by Abrahams and Prince [1962] using neutron diffraction.

NBS lattice constants:

$a = 6.412(1)\text{\AA}$

$b = 7.403(1)$

$c = 3.3025(6)$

$\beta = 99.46(1)^\circ$

Density

(calculated) 2.954 g/cm^3

Reference intensity

I/I_{corundum} 2.5

Additional patterns

1. PDF card 6-143 [Wheeler and Haendler, 1954].

References

Abrahams, S. C. and Prince, E. (1962). J. Chem. Phys. 36, 50.
Wheeler, C.M.Jr. and Haendler, H.M. (1954). J. Am. Chem. Soc. 76, 263.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
4.805	100	110	18.45
3.700	30	020	24.03
3.164	17	200	28.18
3.113	15	101	28.65
2.983	12	011	29.93
2.717	45	101	32.94
2.404	<1	220	37.37
2.353	15	211	38.22
2.299	20	130	39.16
2.191	8	121	41.16
2.023	15	211	44.77
1.968	6	031	46.08
1.919	13	301	47.32
1.850	11	040	49.20
1.750	6	231	52.24
1.704	5	321	53.75
1.650	2	301	55.64
1.629	<1	002	56.44
1.601	12	231	57.51
1.5818	5	400	58.28
1.5556	4	202	59.36
1.5299	6	141	60.46
1.5079	<1	321	61.44
1.4930	2	411	62.12
1.4906	<1	022	62.23
1.4544	<1	420	63.96
1.4413	<1	150	64.61
1.4342	<1	222	64.97
1.3685	1	132	68.51
1.3598	<1	202	69.01
1.3325	4	341	70.63

Europium phosphate, EuPO_4

Sample

The sample was made by I. Mayer [Hebrew University, Jerusalem]. A mixture of $(\text{NH}_4)_2\text{HPO}_4$ and Eu_2O_3 was heated at 500 °C for 2 hours, then at 1100 °C overnight.

Color

Colorless

Structure

Monoclinic, $\text{P2}_1/\text{n}$ (14), $Z=4$, isostructural with monazite [Feigelson, 1964]. The structure of monazite was determined by Kokkoros [1942].

NBS lattice constants:.

$a = 6.6684(5)\text{\AA}$

$b = 6.8671(5)$

$c = 6.3534(5)$

$\beta = 103.94(1)^\circ$

Density

(calculated) 5.808 g/cm^3

Additional patterns

1. PDF card 18-506 [Bril and Wanmaker, 1964]

References

- Bril, A. and Wanmaker, W.L. (1964). J. Electrochem. Soc. 111, 1363.
Kokkoros, P. (1942). Prakt. Akad. Anthenon 17, 163.
Feigelson, R.S. (1964). J. Am. Ceram. Soc. 47, 257.

Internal standard W, $a = 3.16516\text{\AA}$

$\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25 °C

$d\text{ (\AA)}$	I	hkl	$2\theta(^\circ)$
5.127	12	$\bar{1}01$	17.28
4.714	9	110	18.81
4.593	25	011	19.31
4.107	40	$\bar{1}11$	21.62
4.008	18	101	22.16
3.461	17	111	25.72
3.435	15	020	25.92
3.237	55	200	27.53
3.084	7	002	28.93
3.034	100	120	29.41
3.000	5	021	29.76
2.928	15	210	30.51
2.901	6	$\bar{2}11$	30.80
2.813	85	$\bar{1}12, 012$	31.79
2.561	25	202	35.01
2.446	2	211	36.71
2.399	18	$\bar{2}12$	37.45
2.395	19	112	37.52
2.355	6	220	38.18
2.342	1	221	38.41
2.296	5	$\bar{1}22, 022$	39.21
2.208	3	$\bar{3}01$	40.83
2.146	25	031	42.07
2.112	25	$\bar{1}03$	42.79
2.104	25	$\bar{3}11$	42.96
2.081	19	221	43.44
2.058	2	310	43.96
2.053	3	222	44.08
1.988	2	131	45.60
1.923	35	212	47.22
1.899	6	301	47.87
1.868	3	230	48.70
1.862	14	$\bar{2}31$	48.88
1.839	25	$\bar{1}32, 032$	49.53
1.835	15	103	49.64
1.827	15	320	49.87
1.7988	2	$\bar{1}23$	50.71
1.7737	2	113	51.48
1.7638	11	023	51.79
1.7339	19	$\bar{3}22$	52.75
1.7227	4	231	53.12
1.7170	5	040	53.31
1.7043	25	$132, \bar{2}23$	53.74
1.6593	11	140	55.32
1.6377	1	$\bar{1}41$	56.49
1.6180	4	$123, 400$	56.86
1.6002	7	402	57.55
1.5782	2	141	58.43
1.5750	7	410	58.56
1.5701	7	330	58.76

Europium phosphate, EuPO_4 – continued

$d \text{ (Å)}$	I	hkl	$2\theta(^{\circ})$
1.5583	2	$\bar{4}12$	59.25
1.5547	4	312	59.40
1.5476	2	$\bar{1}14$	59.70
1.5420	5	004	59.94
1.5322	2	213	60.36
1.5288	1	033, $\bar{3}23$	60.51
1.5168	3	240	61.04
1.5101	5	$\bar{3}32$	61.34
1.5059	10	$\bar{2}14$	61.53
1.5003	4	$\bar{1}42, 042$	61.78
1.4503	2	$\bar{4}22$	64.16
1.4473	1	322, $\bar{4}11$	64.31
1.4417	4	$\bar{1}24$	64.59
1.4358	3	241	64.89
1.4322	2	133	65.07
1.4295	3	223	65.21
1.4260	3	$\bar{2}42$	65.39
1.4062	1	024	66.43
1.3974	3	$\bar{3}14$	66.90
1.3591	2	421	69.05
1.3473	4	$\bar{4}31$	69.74
1.3434	5	150, $\bar{3}40$	69.97
1.3379	3	$\bar{4}23$	70.30
1.3320	3	$\bar{1}43$	70.66
1.3263	2	$\bar{1}51$	71.01
1.3179	4	$\bar{3}24, 043$	71.53
1.3152	7	124	71.70
1.3091	11	332, $\bar{4}02$	72.09
1.3052	10	$\bar{3}42, \bar{1}34$	72.34

Glucose, D, alpha, (dextrose), $C_6H_{12}O_6$

Sample

The sample was NBS Standard Reference Material 41a. The dextrose was produced by Pfanstiehl Laboratories, Inc. Chicago, Illinois

moisture..... less than 0.02%
ash..... less than 0.01%

Color

Colorless

Structure

Orthorhombic, $P2_12_12_1(19)$. $Z=4$, [Sponsler and Dove, 1931]. The structure was determined by McDonald and Beevers [1952].

NBS lattice constants:

$a = 10.368(2) \text{ \AA}$
 $b = 14.856(2)$
 $c = 4.9808(6)$

Density

(calculated) 1.560 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 2.3$

Additional patterns

1. PDF card 1-374 [Sponsler and Dove, 1931]
2. PDF card 3-228 Inst. of Physics at University College, Cardiff, Wales.

References

- McDonald, T.R.R. and Beevers, C.A. (1952). Acta Cryst. **5**, 654.
Sponsler, O.L. and Dove, W.H. (1931). J. Am. Chem. Soc. **53**, 1639.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ $CuK\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
8.50	7	110	10.40
7.42	6	020	11.91
6.04	15	120	14.66
5.181	14	200	17.10
4.894	1	210	18.11
4.724	20	011	18.77
4.487	4	101	19.77
4.298	100	111	20.65
4.251	8	220	20.88
3.841	4	121	23.14
3.709	1	040	23.97
3.590	4	201	24.78
3.493	11	140,211	25.48
3.366	2	310	26.46
3.326	3	131	26.78
3.234	2	221	27.56
3.132	19	320	28.47
3.018	1	240	29.57
2.977	2	041	29.99
2.907	4	231	30.73
2.856	4	150	31.29
2.833	1	330	31.55
2.789	<1	311	32.06
2.651	2	321	33.78
2.590	5	400	34.60
2.581	4	241	34.73
2.551	4	410,051	35.15
2.530	2	340	35.45
2.489	8	002	36.05
2.477	9	151,060	36.23
2.455	7	012	36.57
2.449	7	420	36.67
2.423	2	102	37.08
2.408	1	160	37.31
2.390	1	112	37.60
2.362	7	022	38.07
2.295	4	430	39.22
2.273	4	411	39.62
2.255	6	341	39.94
2.233	1	260	40.35
2.217	4	061	40.66
2.196	1	421	41.06
2.168	1	161	41.62
2.150	1	222	41.99
2.125	<1	440	42.51
2.085	1	431	43.36
2.080	1	170	43.47
2.053	4	510,351	44.08
2.002	1	312	45.26
1.963	2	270	46.20

Glucose, D, alpha, (dextrose), $C_6H_{12}O_6$ - continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.953	2	450,071	46.47
1.918	2	171	47.36
1.914	2	501,530	47.47
1.899	1	511	47.87
1.867	1	361	48.74
1.854	1	521	49.10
1.827	1	180,271	49.87
1.818	<1	451	50.14
1.809	<1	370	50.40
1.791	2	252,460	50.95
1.786	1	531	51.10
1.775	<1	342	51.43
1.756	1	062	52.05
1.745	<1	422	52.39
1.741	<1	081	52.52
1.716	<1	610,181	53.35
1.701	1	541,550+	53.86
1.684	1	461,620	54.44
1.671	1	352	54.90
1.663	1	262	55.18
1.650	<1	013,281	55.66
1.630	1	190,113	56.39
1.623	1	611	56.65
1.617	<1	442	56.90
1.601	1	123	57.53
1.595	2	172,621	57.75
1.5811	1	203	58.31
1.5664	1	091,640+	58.91

Indium sulfide, In_2S_3

Sample

The In_2S_3 was made by W.S. Brower by heating the elements in a sealed silica tube at 460 °C for sixteen hours and at 880 °C for six hours.

Color

Unground: dark grayish red

Ground: strong reddish brown

Structure

Tetragonal, I4_122 (98), $Z=16$. The structure was studied by Rooymans [1959] and by Goodyear and Steigmann [1961].

NBS lattice constants: °

$a = 7.619(1)\text{Å}$

$c = 32.329(4)$

Density

(calculated) 4.613 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 4.2$

Polymorphism

Hahn and Klinger [1949] found that a low temperature form transformed irreversibly at about 330 °C to a high form which they indexed as cubic with a few extra non-cubic lines.

Additional patterns

1. Goodyear and Steigmann [1961].

References

- Goodyear, J. and Steigmann, G.A. (1961). Proc. Phys. Soc. **78** 491.
Hahn, H. and Klinger, W. (1949). Z. anorg. Chem. **260**, 97.
Rooymans, C.J.M. (1959). J. Inorg. Nucl. Chem. **11**, 78.

Internal standard W, $a = 3.16516 \text{ Å}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ Å}$; temp. 25 °C			
$d (\text{Å})$	I	hkl	$2\theta (^\circ)$
8.09	4	004	10.93
7.40	3	101	11.95
6.21	30	103	14.24
5.110	12	112	17.34
4.927	2	105	17.99
4.041	3	008	21.98
3.947	2	107	22.51
3.811	18	200,116	23.32
3.445	2	204	25.84
3.392	2	211	26.25
3.249	100	109,213	27.43
3.112	12	206	28.66
3.015	1	215	29.60
2.770	3	208,1·1·10	32.29
2.741	3	1·0·11,217	32.64
2.694	50	0·0·12,220	33.23
2.557	1	224	35.07
2.532	1	301	35.42
2.472	4	219,303	36.31
2.382	1	312	37.74
2.364	3	1·0·13,305	38.04
2.309	1	314	38.97
2.225	3	2·1·11,307	40.51
2.199	9	2·0·12,316	41.00
2.123	1	1·1·14	42.54
2.107	2	321	42.88
2.074	45	309,323	43.61
2.009	3	2·1·13,325	45.09
1.905	65	2·2·12,400	47.71
1.845	1	1·0·17,411	49.34
1.8213	6	329,413,+	50.04
1.7766	1	3·0·13,415	51.39
1.7224	1	334,408,+	53.13
1.7161	1	3·2·11,417	53.34
1.7037	3	336,420,+	53.76
1.6673	3	3·1·14,424	55.03
1.6615	3	1·0·19,2·1·17	55.24
1.6429	13	3·0·15,419	55.92
1.6242	5	426,2·0·18	56.62
1.6161	3	2·2·16,0·0·20	56.93
1.5701	2	3·3·10,428	58.76
1.5647	2	4·1·11	58.98
1.5556	10	4·0·12	59.36
1.5224	1	2·1·19,431,+	60.79
1.5090	4	1·0·21,3·2·15	61.39
1.4876	3	2·0·20,512	62.37
1.4835	2	4·1·13,435	62.56
1.4475	1	437	64.30
1.4403	4	3·1·18,516,+	64.66
1.4181	2	1·1·22,3·3·14	65.80

Indium sulfide, In_2S_3 – continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.4137	2	3·0·19,521,+	66.03
1.4028	16	439,523,+	66.61
1.3527	2	4·3·11,527	69.42
1.3470	8	440,0·0·24	69.76
1.3252	1	3·2·19,4·1·17	71.08
1.2746	1	1·0·25,5·2·11	74.36
1.2701	2	2·0·24,536,+	74.67
1.2442	9	4·3·15,613,+	76.50
1.2364	2	4·2·18,606	77.07
1.2301	2	3·0·23,615,+	77.54
1.2119	1	1·1·26,608,+	78.93
1.2046	6	4·4·12,620,+	79.49
1.1895	1	4·3·17,541	80.72
1.1829	1	1·0·27,619,+	81.26
1.1728	1	4·2·20	82.11
1.1524	1	3·0·25,547,+	83.89
1.1488	1	5·1·18,6·0·12	84.21
1.1294	5	549,633,+	86.00
1.1190	1	4·1·23,635,+	87.00
1.0997	14	4·0·24,6·2·12	88.93
1.0832	<1	3·0·27,639,+	90.65
1.0566	2	556,640,+	93.61
1.0462	2	6·1·17,721	94.83
1.0418	7	3·2·27,709,+	95.36
1.0368	4	6·0·18,646,+	95.97
1.0334	3	1·0·31,725,+	96.38
1.0223	1	5·5·10,648,+	97.79
1.0048	1	6·3·15,729	100.10
0.9715	2	7·0·15,653,+	104.91
.9524	4	4·4·24,800	107.96
.9413	1	659,743,+	109.83

Iron chloride hydrate, $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by permitting anhydrous FeCl_2 to hydrate in humid air. The sample was somewhat hygroscopic.

Color

light yellowish brown

Structure

Monoclinic, $C2/m$ (12), $Z=2$, isostructural with $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$ and $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$. The structure was determined by Morosin and Graeber [1965].

NBS lattice constants:
 $a = 7.3523(6) \text{ \AA}$
 $b = 8.5609(8)$
 $c = 3.6367(3)$
 $\beta = 98.10(1)^\circ$

Density

(calculated) 2.385 g/cm^3

Additional patterns

- PDF card 1-210 [Hanawalt et al., 1938]

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.
 Morosin, B. and Graeber, E. J. (1965). J. Chem. Phys. **42**, 898.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
5.548	100	110	15.96
4.281	75	020	20.73
3.641	7	200	24.43
3.600	7	001	24.71
3.181	8	$\bar{1}11$	28.03
2.884	45	111	30.98
2.773	45	220	32.25
2.763	90	$\bar{2}01$	32.38
2.657	25	130	33.70
2.396	45	201	37.50

$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
2.335	12	310	38.53
2.321	25	$\bar{2}21$	38.77
2.193	5	131	41.13
2.141	35	040	42.18
2.092	45	$\bar{3}11, 221$	43.21
2.088	35	131	43.30
1.848	7	330, 311	49.26
1.840	6	041	49.51
1.820	19	400	50.09
1.800	13	002	50.67
1.769	14	$\bar{1}12$	51.62
1.721	9	$\bar{3}31$	53.18
1.711	7	202	53.49
1.692	20	$\bar{2}41$	54.17
1.674	11	420	54.79
1.6668	9	150	55.05
1.6609	8	112	55.26
1.6593	7	022	55.32
1.5959	18	241	57.72
1.5772	4	331	58.47
1.5313	4	$\bar{1}51$	60.40
1.5270	7	$\bar{1}32$	60.59
1.4943	6	151	62.06
1.4485	3	421	64.25
1.4352	4	510	64.92
1.4268	5	060	65.35
1.3987	3	350	66.83
1.3863	9	440	67.51
1.3775	8	042	68.00
1.3408	6	$\bar{3}51, 312$	70.13
1.3263	<4	061	71.01
1.3138	<4	$\bar{4}22$	71.79
1.2966	<4	530	72.89
1.2739	<4	511	74.41
1.2693	<4	351	74.72
1.2677	4	$\bar{2}61$	74.83
1.2432	4	152	76.57
1.2254	4	261, 332	77.89
1.2065	4	$\bar{5}12, 170$	79.35
1.2021	4	601	79.70
1.1981	4	402	80.02
1.1906	<4	203	80.63
1.1741	<4	531	82.00
1.1605	4	442	83.17
1.1572	4	621	83.46
1.1536	4	422	83.78
1.1481	4	113	84.28
1.1472	4	$\bar{2}23$	84.36
1.1357	<4	171	85.41
1.1317	<4	$\bar{3}13$	85.78

Lead bromide chloride, PbBrCl

Sample

The sample was prepared by melting a 1:1 mixture of PbCl₂ and PbBr₂. The sample was then ground and annealed in a sealed glass tube at 400 °C overnight.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z=4, isostructural with BaCl₂. There is a complete solid solution series between PbBr₂ and PbCl₂ [Calingaert et al., 1949]. The structure of PbCl₂ was determined by Bräkken and Harang [1928].

NBS lattice constants:

a = 7.801(1) Å

b = 9.207(1)

c = 4.5803(5)

Density

(calculated) 6.512 g/cm³

Reference intensity

I/I_{corundum} = 2.0

References

Bräkken, H. and Harang, L. (1928). Z. Krist. 68, 123.

Calingaert, G., Lamb, F.W., and Meyers, F. (1949). J. Am. Chem. Soc. 71, 3712.

Internal standard Ag, a = 4.08641 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	2θ (°)
5.949	2	110	14.88
4.607	6	020	19.25
4.101	17	011	21.65
3.964	80	120	22.41
3.897	30	200	22.80
3.632	90	111	24.49
2.998	30	121	29.78
2.976	20	220	30.00
2.856	16	130	31.29
2.826	100	211	31.64
2.550	50	031	35.17
2.503	8	310	35.84
2.496	3	221	35.95
2.423	16	131	37.07
2.302	40	040	39.09
2.291	40	002	39.30
2.264	40	320	39.78
2.207	10	140	40.85
2.196	40	311	41.06
2.134	40	231	42.32
2.051	1	022	44.12
2.030	1	321	44.61
1.982	30	122,240	45.74
1.949	10	400	46.55
1.908	1	410	47.63
1.821	1	331,241	50.05
1.815	5	222	50.22
1.795	1	420,401	50.83
1.7922	3	150	50.91
1.7869	4	132	51.07
1.7616	2	411	51.86
1.7239	1	340	53.08
1.7090	1	051	53.58
1.6895	3	312	54.25
1.6682	16	151	55.00
1.6229	10	042	56.67
1.6102	20	322	57.16
1.5896	3	142	57.97
1.5647	3	251	58.98
1.5488	7	431	59.65
1.5348	2	060	60.25
1.5052	8	013,160	61.56
1.4984	6	332,242	61.87
1.4874	6	440	62.38
1.4846	10	402	62.51
1.4786	9	113	62.79
1.4663	1	412	63.38
1.4581	12	511	63.78
1.4278	16	260,351	65.30
1.4245	4	123	65.47

Lead bromide chloride, PbBrCl – continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.4111	1	152	66.17
1.4052	8	213	66.48
1.3770	1	342	68.03
1.3672	6	033	68.58
1.3463	2	252,133	69.80
1.3310	4	531	70.72
1.3216	1	360	71.30
1.3030	4	313	72.48
1.2900	5	233	73.33
1.2751	1	062	74.33
1.2639	5	071	75.10
1.2580	3	162	75.51
1.2479	3	171,442	76.23
1.2416	4	522	76.69
1.2395	3	611	76.84
1.2119	6	262	78.93
1.2025	2	271,403	79.67
1.1920	1	413	80.51
1.1626	3	153	82.99
1.1586	2	631	83.34

Magnesium bromide hydrate, $\text{MgBr}_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by treating MgCO_3 with a slight excess of an aqueous solution of HBr and evaporating at about 80°C . The first crystals formed were used.

Color

Colorless

Structure

Monoclinic, C2/m (12), $Z = 2$, isostructural with $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$. The structure was determined by Andress and Gundermann [1934].

NBS lattice constants:

$a = 10.286(1)\text{\AA}$
 $b = 7.331(1)$
 $c = 6.211(1)$
 $\beta = 93.34(1)^\circ$

Density

(calculated) 2.076 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 2.9$

Additional patterns

1. PDF card 1-1045 [Hanawalt et al., 1938].

References

Andress, K.R. and Gundermann, J. (1934). Z. Krist. 87A, 345.
 Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938) Ind. Eng. Chem. Anal. Ed. 10, 457.

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25°C			
$d\text{ (\AA)}$	I	hkl	$2\theta(^\circ)$
6.20	10	001	14.28
5.133	5	200	17.26
4.375	2	111	20.28
4.225	100	111	21.01
4.070	40	201	21.82
3.844	2	201	23.12
3.664	35	020	24.27
3.154	10	021	28.27
3.101	40	310,002	28.77
2.982	30	220	29.94
2.835	18	311	31.53
2.791	30	112	32.04
2.724	70	202,221	32.85
2.717	55	311,112	32.94
2.655	3	221	33.73
2.589	1	202	34.62
2.568	1	400	34.91
2.423	5	401	37.08
2.378	6	130	37.80
2.368	7	022	37.97
2.325	14	401	38.70
2.254	1	312	39.97
2.210	9	131	40.79
2.187	1	222	41.25
2.136	4	312	42.27
2.114	6	222	42.73
2.067	1	003	43.77
2.037	3	402	44.44
2.021	3	421	44.80
1.989	4	330	45.58
1.973	4	113	45.95
1.963	4	421	46.20
1.958	4	203	46.34
1.933	2	113	46.98
1.915	8	511	47.43
1.899	12	132	47.86
1.879	6	203	48.39
1.875	10	331,132	48.51
1.8543	2	511	49.09
1.8329	4	040	49.70
1.8004	2	023	50.66
1.7804	7	422	51.27
1.7634	4	313	51.80
1.7266	3	223,240	52.99
1.7117	3	600,512	53.49
1.7034	2	422	53.77
1.6792	3	313	54.61
1.6718	6	223,241	54.87
1.6576	2	403	55.38
1.6486	2	332	55.71

Magnesium bromide hydrate, $\text{MgBr}_2 \cdot 6\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	2θ (°)
1.6261	2	512,601	56.55
1.5720	2	530	58.68
1.5667	2	403	58.90
1.5504	5	620,004	59.58
1.5403	5	531	60.01
1.5213	2	$\bar{2}42$	60.84
1.5128	4	$\bar{1}14$	61.22
1.5085	3	$\bar{2}04,531$	61.41
1.4958	1	242	61.99
1.4861	2	621	62.44
1.4609	2	$\bar{4}41,204$	63.64
1.4581	2	$\bar{3}33$	63.78
1.4391	4	441	64.72
1.4280	2	$\bar{5}32,024$	65.29
1.4189	2	$\bar{7}11$	65.76
1.4156	1	$\bar{1}51$	65.93
1.4103	2	151	66.21
1.3906	1	513	67.27
1.3776	<1	532	67.99
1.3625	2	$\bar{4}04,442$	68.85
1.3573	3	$\bar{6}03,224$	69.15
1.3475	2	350	69.73
1.3381	1	243	70.29
1.3341	2	$\bar{7}12$	70.53
1.3231	1	351	71.21
1.3189	<1	$\bar{1}52$	71.47
1.3120	2	243	71.90
1.3106	1	351,152	71.99

Magnesium chloride hydrate (bischofite), $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by boiling a saturated aqueous solution of MgCl_2 and filtering off the crystals. The sample was somewhat hygroscopic.

Color

Colorless

Optical data

Biaxial (+), $N_\alpha=1.498$, $N_\beta=1.505$, $N_\gamma=1.525$. 2V is large.

Structure

Monoclinic, C2/m (12), Z = 2, isostructural with $\text{MgBr}_2 \cdot 6\text{H}_2\text{O}$. The structure of bischofite was determined by Andress and Gundermann [1934].

NBS lattice constants:

a = 9.871(2) Å
b = 7.113(1)
c = 6.079(1)
β = 93.74(1)

Density

(calculated) 1.585 g/cm³

Reference intensity

I/I_{corundum} = 0.8

Additional patterns

1. PDF card 1-431 [Hanawalt et al., 1938].

References

Andress, K.R. and Gundermann, J. (1934). Z. Krist. 87A, 345.
Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Internal standard Ag, a = 4.08641 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	2θ (°)
5.77	17	110	15.34
4.263	20	111	20.82
4.101	100	111	21.65
3.955	30	201	22.46
3.708	10	201	23.98
3.556	30	020	25.02
3.068	2	021	29.08
3.032	5	002	29.43
2.981	35	310	29.95
2.883	65	220	30.99
2.740	35	311	32.66
2.728	55	112	32.80
2.661	8	202	33.65
2.643	90	221, 112	33.89
2.616	7	311	34.25
2.567	9	221	34.92
2.463	7	400	36.45
2.336	9	401	38.50
2.308	25	022, 130	38.99
2.232	30	401	40.38
2.192	2	312	41.15
2.167	5	131	41.65
2.145	8	131	42.10
2.131	3	222	42.39
2.065	8	312	43.80
2.051	11	222	44.11
1.952	2	421	46.49
1.922	5	330	47.25
1.914	7	203	47.46
1.890	6	421	48.10
1.849	35	132	49.25
1.844	20	511	49.38
1.830	6	203	49.79
1.812	7	331	50.32
1.778	15	040	51.35
1.757	5	023	52.00
1.7272	13	422	52.97
1.7218	11	313	53.15
1.6860	4	223	54.37
1.6418	3	600	55.96
1.6221	6	241	56.70
1.5964	5	332	57.70
1.5088	4	133	61.40
1.4874	12	531	62.38

Manganese chloride hydrate, $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by heating a solution of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ in ethyl alcohol. Excess alcohol was removed by pressing between filter papers.

Color

Light pink

Optical data

Biaxial (+), $N_\alpha = 1.583$, $N_\beta = 1.613$, $N_\gamma = 1.664$; 2V is very large.

Structure

Monoclinic, $C2/m$ (12), $Z=2$ [Neuhaus, 1937], iso-structural with $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$. The structure was determined by Vainshtein [1952].

NBS lattice constants:

$a = 7.4062(5) \text{ \AA}$
 $b = 8.8032(5)$
 $c = 3.6881(5)$
 $\beta = 98.22(1)^\circ$

Density

(calculated) 2.259 g/cm^3

Reference intensity

$I/I_{\text{copper}} = 2.3$

Additional patterns

1. PDF card 1-199 [Hanawalt et al., 1938].
2. PDF card 3-743 [Neuhaus, 1937].

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938).
 Ind. Eng. Chem. Anal. Ed. 10, 457.
 Neuhaus, A. (1937). Z. Krist. 98, 112.
 Vainshtein, B.K. (1952). Dokl. Akad. Nauk SSSR 83, 227.

Internal standard W, $a = 3.16516 \text{ \AA}$

$\text{CuK}\alpha_1$, $\lambda = 1.54056 \text{ \AA}$; temp. 25°C

$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.636	100	110	15.71
4.399	65	020	20.17
3.667	3	200	24.25
3.227	4	111	27.62
2.922	25	111	30.57
2.817	30	220	31.74
2.794	45	201	32.01
2.725	14	130	32.84
2.419	25	201	37.13
2.355	16	$\bar{2}21, 310$	38.19

$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
2.202	19	040	40.96
2.130	13	131	42.41
2.120	20	221	42.61
2.116	18	311	42.70
1.887	1	240	48.19
1.878	2	330	48.43
1.866	2	311	48.75
1.833	9	400	49.71
1.8250	8	002	49.92
1.7945	7	$\bar{1}12$	50.84
1.7499	4	$\bar{3}31$	52.23
1.7287	9	$\bar{2}41$	52.92
1.7120	2	150	53.48
1.6918	5	420	54.17
1.6282	9	241	56.48
1.6004	<1	331	57.54
1.5547	3	$\bar{1}32$	59.40
1.5304	2	151	60.44
1.4673	1	060	63.33
1.4463	1	510	64.36
1.4285	1	350	65.25
1.4084	6	440	66.31
1.3695	2	$\bar{3}51$	68.45
1.3618	1	260, 061	68.89
1.3116	<1	530	71.93
1.2988	1	$\bar{2}61$	72.75
1.2841	1	511	73.72
1.2545	1	261	75.76
1.2393	1	$\bar{1}70$	76.86
1.2118	1	601	78.94
1.2096	1	402	79.11
1.1867	<1	531	80.95
1.1771	1	620	81.75
1.1682	3	$\bar{6}21$	82.50
1.1654	2	171	82.75
1.1453	2	460	84.53
1.1363	1	$\bar{5}32$	85.36
1.1266	<1	550	86.27
1.1181	1	370	87.09
1.1116	1	601, $\bar{5}51$	87.73
1.1002	<1	080	88.87
1.0893	1	$\bar{3}71$	90.00
1.0777	<1	621	91.24
1.0658	1	461	92.56
1.0615	1	641	93.05
1.0396	<1	710, $\bar{7}11$	95.62
1.0372	1	$\bar{1}72$	95.92
1.0239	<1	281	97.58
1.0096	1	552	99.45
0.9923	1	641	101.84
.9862	<1	730, $\bar{7}31$	102.71

Mercury ammine chloride, $\text{Hg}(\text{NH}_3)_2\text{Cl}_2$

Sample

The sample was prepared by exposing finely ground HgCl_2 to NH_3 gas in a previously evacuated desiccator.

Color

Colorless

Structure

Cubic, $Z=1/2$, structure determined by MacGillavry and Bijvoet [1936].

NBS lattice constant: $a = 4.053(2)\text{\AA}$

Density

(calculated) 3.809 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 1.6$

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25°C			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
2.868	17	110	31.16
2.342	100	111	38.41
2.028	70	200	44.65
1.4332	25	220	65.02
1.2220	19	311	78.15
1.1699	8	222	82.36

Additional patterns

1. MacGillavry and Bijvoet [1936]

References

MacGillavry, C. H. and Bijvoet, J. M. (1936). *Z. Krist.* **94**, 231.

Neodymium phosphate, NdPO₄

Sample

The sample was made by I. Mayer [Hebrew University, Jerusalem]. A mixture of (NH₄)₂HPO₄ and Nd₂O₃ was heated at 500 °C for 2 hours, then at 1100 °C overnight.

Color

Pale purplish pink

Structure

Monoclinic, P2₁/n (14), Z=4, isostructural with monazite. The structure of NdPO₄ was determined by Mooney [1948].

NBS lattice constants:

a = 6.7441(6) Å

b = 6.9584(7)

c = 6.4111(7)

β = 103.67(1)°

Density

(calculated) 5.435 g/cm³

Reference intensity

I/I_{corundum} = 1.0

Polymorphism

NdPO₄ occurs also in a low temperature modification, which may require some zeolite water for stabilization [Mooney, 1950]. PDF card 4-644 is of this form.

Additional patterns

1. Weigel et al. [1965]

References

- Mooney, R.C.L. (1948). J. Chem. Phys. **16**, 1003.
Mooney, R.C.L. (1950). Acta Cryst. **3**, 337.
Weigel, von F., Sherer, V. and Henschel, H. (1965) Radiochimica Acta **4**, 18.

Internal standard W, a = 3.16516 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	2θ (°)
5.17	14	$\bar{1}01$	17.13
4.78	10	110	18.56
4.645	25	011	19.09
4.151	45	$\bar{1}11$	21.39
4.064	16	101	21.85
3.508	19	111	25.37
3.479	18	020	25.58
3.277	60	200	27.19
3.116	8	002	28.62
3.072	100	120	29.04
3.040	7	021	29.36
2.965	17	210	30.12
2.933	5	$\bar{2}11$	30.45
2.842	100	012, $\bar{1}12$	31.45
2.583	25	$\bar{2}02$	34.70
2.479	<1	211	36.21
2.423	25	112, $\bar{2}12$	37.08
2.385	7	220	37.68
2.368	2	$\bar{2}21$	37.97
2.321	6	022, $\bar{1}22$	38.77
2.233	3	$\bar{3}01$	40.36
2.187	3	130	41.24
2.174	25	031	41.51
2.129	40	$\bar{1}03$	42.43
2.126	40	$\bar{3}11$	42.48
2.109	25	221	42.84
2.085	3	310	43.36
2.075	3	122, $\bar{2}22$	43.58
2.038	1	$\bar{1}13$	44.42
2.015	2	131	44.95
1.991	<1	013	45.53
1.949	35	212	46.55
1.924	9	301	47.19
1.892	1	$\bar{2}30$	48.04
1.885	16	231	48.25
1.860	35	032, $\bar{1}32$	48.93
1.851	19	320	49.19
1.8165	2	$\bar{1}23$	50.18
1.7945	2	113	50.84
1.7834	11	023	51.18
1.7521	20	$\bar{3}22$	52.16
1.7400	7	040	52.55
1.7266	25	132, $\bar{2}32$	52.99
1.7215	20	303	53.16
1.6812	12	140	54.54
1.6715	1	$\bar{3}13$	54.88
1.6494	1	$\bar{1}41$	55.68
1.6383	6	123, 400	56.09
1.6159	9	402	56.94
1.5989	2	141	57.60

Neodymium phosphate, NdPO_4 – continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.5949	9	410	57.76
1.5903	8	330	57.94
1.5757	5	312	58.53
1.5616	3	$\bar{1}14$	59.11
1.5573	6	004, $\bar{2}04$	59.29
1.5427	<1	$\bar{3}23$	59.91
1.5364	3	240	60.18
1.5267	6	$\bar{3}32$	60.60
1.5193	13	$\bar{2}14, 042$	60.93
1.4820	<1	420	62.63
1.4659	3	411, $\bar{4}22$	63.40
1.4554	6	$\bar{1}24, 241$	63.91
1.4477	4	223	64.29
1.4431	4	142, $\bar{2}42$	64.52
1.4214	1	024, $\bar{2}24$	65.63
1.4092	3	$\bar{3}14$	66.27
1.3768	4	421	68.04
1.3636	5	$\bar{4}31$	68.79
1.3605	5	150, 340	68.97
1.3534	2	303	69.38
1.3507	3	$\bar{4}23$	69.54
1.3470	3	$\bar{1}43$	69.76
1.3436	3	$\bar{1}51$	69.96
1.3332	5	043	70.59
1.3292	11	$\bar{3}24, 313$	70.83
1.3270	13	332, 402	70.97
1.3237	6	$\bar{5}11$	71.17
1.3200	8	$\bar{3}42$	71.40
1.3187	8	$\bar{1}34$	71.48
1.3125	2	233	71.87
1.3063	2	$\bar{2}43$	72.27
1.3030	5	412	72.48
1.2927	5	034, $\bar{2}34, +$	73.15
1.2880	3	510	73.46
1.2805	2	250, $\bar{1}05$	73.96
1.2701	12	$\bar{1}52, \bar{4}14, +$	74.67
1.2595	4	$\bar{1}15, 431$	75.41
1.2495	2	$\bar{5}03$	76.12
1.2382	6	$\bar{5}22$	76.94
1.2300	<1	513	77.55
1.2254	8	501, 152	77.89
1.2228	12	$\bar{3}34$	78.09
1.2123	2	224	78.90

Nickel chloride hydrate, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of NiCl_2 (Fisher Scientific Co.). Because of the platy nature and the instability of the material, the intensity values are subject to some error.

Color

Deep yellowish green

Optical data

Biaxial (+) $N_\alpha=1.590$, $N_\beta=1.620$, $N_\gamma=1.648$; 2V is very large.

Structure

Monoclinic, $I2/m$ (12), $Z = 2$, isostructural with $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$. The structure was determined by Mizuno (1961).

NBS lattice constants:

$a = 8.786(2)\text{\AA}$
 $b = 7.076(2)$
 $c = 6.625(2)$
 $\beta = 97.21(1)^\circ$

Density

(calculated) 1.932 g/cm^3

Additional patterns

1. PDF card 1-200 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn, R.W., and Frevel, L.K. (1938).
 Ind. Eng. Chem. Anal. Ed. **10**, 457.
 Mizuno, J. (1961). J. Phys. Soc. Japan **16**, 1574.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
5.59	100	$\bar{1}01$	15.83
5.50	40	110	16.10
4.96	12	101	17.88
4.82	35	011	18.39
4.360	2	200	20.35
3.542	10	020	25.12
3.392	2	$\bar{2}11$	26.25
3.288	1	002	27.10
3.095	4	211	28.82
2.994	9	$\bar{1}21$	29.82
2.926	35	$\bar{1}12$	30.53
2.799	17	$\bar{2}02$	31.95
2.747	30	220	32.57
2.729	5	112	32.79
2.689	20	310	33.29
2.543	8	301	35.27
2.407	16	022	37.32
2.220	3	031	40.60
2.211	2	$\bar{3}12$	40.77
2.192	5	$\bar{1}03, 321$	41.14
2.178	20	400	41.42
2.065	3	$103, 321$	43.81
2.057	7	411	43.98
2.030	4	222	44.59
2.013	1	$\bar{2}31$	45.00
1.980	3	$\bar{2}13$	45.80
1.971	8	312	46.00
1.932	3	402	47.00
1.921	3	411	47.29
1.900	10	$\bar{1}32$	47.83
1.862	5	$\bar{1}23$	48.85
1.856	5	420	49.03
1.832	2	330	49.74
1.783	1	123	51.20
1.695	7	422	54.07
1.687	3	$\bar{1}41$	54.35
1.636	1	501	56.17
1.6084	3	$\bar{1}14, 413$	57.23
1.6045	6	$\bar{2}04, 033$	57.38
1.5888	3	431	58.00
1.5853	3	$\bar{5}12$	58.14
1.5609	2	$\bar{5}21$	59.14
1.5575	2	042	59.28
1.5483	4	332	59.67
1.4969	2	323	61.94
1.4774	1	204	62.85
1.4628	2	$233, \bar{2}24$	63.55
1.4558	2	503	63.89
1.4514	2	341	64.11

Nickel fluoride hydrate, $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was made by slow evaporation at room temperature of an aqueous solution of NiF_2 with a slight excess of HF.

Color

Brilliant yellow green

Structure

Orthorhombic, $P2_1ab$ (29), $Z=4$, isostructural with $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$. The space group and cell parameters of $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ were determined by Rao et al. [1965].

NBS lattice constants:

$a = 7.485(2)\text{\AA}$
 $b = 12.482(2)$
 $c = 5.272(1)$

Density

(calculated) 2.276 g/cm^3

Reference intensity

I/I_{corundum} 2.0

Polymorphism

Easwaran and Srinivasan [1965] reported, by comparison of powder patterns, that $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ was isostructural with $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$. However, Penfold and Taylor [1960] reported $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ as rhombohedral. This suggests a second form of $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ exists.

Additional patterns

1. PDF card 1-267 [Hanawalt et al., 1938]

References

- Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.
 Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. 13, 953.
 Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. 3, 68.

Internal standard Ag, $a = 4.08641\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25°C			
$d\text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.28	6	001	16.78
4.857	85	011	18.25
4.795	100	120	18.49
4.075	50	111	21.79
3.748	6	200	23.73
3.546	3	121	25.09
3.266	3	031	27.28
3.120	30	040	28.59
3.052	4	201	29.24
2.964	35	211	30.13
2.741	15	221	32.64
2.637	1	002	33.97
2.580	3	012	34.74
2.528	8	141	35.48
2.460	3	231	36.49
2.439	6	112	36.82
2.309	4	122	38.98
2.256	1	051	39.93
2.219	8	311	40.62
2.155	25	202	41.89
2.124	4	212	42.53
2.037	1	222	44.43
2.004	13	160	45.22
1.982	3	331	45.74
1.933	9	251	46.98
1.913	3	232	47.49
1.871	5	400	48.61
1.828	1	341	49.85
1.793	5	312,420	50.90
1.773	10	242	51.51
1.740	13	013,322	52.56
1.719	1	261	53.24
1.689	2	071	54.25
1.674	1	351	54.81
1.661	2	332	55.25
1.648	4	171	55.72
1.6311	3	252	56.36
1.6050	2	440	57.36
1.5974	3	360	57.66
1.5951	2	162	57.75
1.5821	2	133	58.27
1.5787	1	213	58.41
1.5607	1	080	59.15

Potassium bromide iodide, $\text{KBr}_{.33}\text{I}_{.67}$

Sample

The sample was prepared by melting a 1:2 mixture of KBr and KI. After grinding, it was annealed at 450 °C overnight.

Color

Colorless

Optical data

Isotropic, $N=1.633$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, NaCl type. There is a complete solid solution series from KBr to KI [Wrzesnewsky, 1912].

NBS lattice constant:

$$a = 6.9174(3) \text{ \AA}$$

Density

(calculated) 3.02 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 8.4$

References

Wrzesnewsky, J.B. (1912). Z. anorg. Chem. **74**, 110.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ CuK α_1 , $\lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
3.997	25	111	22.22
3.456	100	200	25.76
2.446	40	220	36.71
2.086	10	311	43.35
1.997	10	222	45.37
1.7290	7	400	52.91
1.5868	2	331	58.08
1.5464	10	420	59.75
1.4118	5	422	66.13
1.3312	1	511	70.71
1.2227	1	440	78.10
1.1694	1	531	82.40
1.1528	2	600	83.85
1.0935	1	620	89.56
1.0549	<1	533	93.81
1.0428	<1	622	95.24
.9985	<1	444	100.96
.9687	<1	711	105.34
.9592	<1	640	106.85
.9245	<1	642	112.85
.9006	<1	731	117.58
.8388	<1	800	133.34

Potassium bromide iodide, $\text{KBr}_{.67}\text{I}_{.33}$

Sample

The sample was prepared by melting together KBr and KI in a 2:1 molar ratio. After grinding the sample was heated at 400 °C overnight.

Color

Colorless

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z = 4$, NaCl type. There is a complete solid solution series between KBr and KI [Wrzesnewsky, 1912].

NBS lattice constant:

$$a = 6.7624(3)\text{\AA}$$

Density

(calculated) 2.90 g/cm^3

Reference intensity

I/I_{corundum} 8.4.

Optical data

Isotropic, $N=1.597$

References

Wrzesnewsky, J.B. (1912). Z. anorg. Chem. 74, 110.

Internal standard W, $a = 3.16516\text{\AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{\AA}$; temp. 25 °C			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
3.909	15	111	22.73
3.380	100	200	26.35
2.390	30	220	37.60
2.040	5	311	44.38
1.952	7	222	46.48
1.691	5	400	54.19
1.5514	2	331	59.54
1.5125	7	420	61.23
1.3805	3	422	67.83
1.3014	1	511	72.58
1.1959	1	440	80.20
1.1431	<1	531	84.73
1.1273	1	600	86.20
1.0693	1	620	92.17
1.0193	<1	622	98.17
.9760	<1	444	104.22
.9467	<1	711	108.90
.9377	<1	640	110.46
.9036	<1	642	116.97
.8805	<1	731	122.04
.8453	<1	800	131.36
.8200	<1	820	139.88

Potassium cobalt fluoride, K_2CoF_4

Sample

The sample was prepared by treating a 1:1 mixture of K_2CO_3 and $CoCO_3$ with HF, drying, and heating the product for 10 minutes at 400 °C, followed by 10 minutes at 750 °C.

Color

Medium pink

Structure

Tetragonal, $I4/mmm$ (139), $Z=2$, isostructural with K_2MgF_4 and similar tetrafluorides [Rüdorff et al., 1959]. The structure of K_2MgF_4 was determined by Brehler and Winkler [1954].

NBS lattice constants:

$$a = 4.0750(4) \text{ \AA}$$

$$c = 13.089(1)$$

Density

(calculated) 3.256 g/cm³

Reference intensity

I/I_{corundum} 3.4

Major impurities

~ .05% Ag, Ca, Cu, Fe, Ni, Zn and Si.

~ .5% Al

References

- Brehler, B. and Winkler, H.G.F. (1954). Heidelberg Beitr. Mineral. Petrog. 4, 6.
 Rüdorff, W., Kändler, J., Lincke, G., and Babel, D. (1959). Angew. Chem. 71, 672.

Internal standard W, $a = 3.16516 \text{ \AA}$ $CuK\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d \text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
6.53	100	002	13.54
3.890	8	101	22.84
3.272	1	004	27.23
2.976	40	103	30.00
2.879	30	110	31.04
2.637	2	112	33.97
2.202	10	105	40.95
2.181	40	006	41.36
2.163	10	114	41.72
2.038	25	200	44.42
1.946	3	202	46.64
1.806	1	211	50.49
1.7394	7	116	52.57
1.6814	8	213	54.53
1.6364	5	008	56.16
1.4956	3	215	62.00
1.4891	9	206	62.30
1.4403	4	220	64.66
1.4229	1	118	65.55
1.3697	1	109	68.44
1.3089	<1	0·0·10	72.10
1.2970	1	303	72.87
1.2884	2	310	73.43
1.2756	2	208	74.29
1.2058	1	305	79.41
1.2022	2	226	79.69
1.1919	1	1·1·10	80.52
1.1421	1	1·0·11	84.82
1.1365	1	219	85.34
1.1097	1	316	87.92

Potassium tungsten oxide, K_2WO_4

Sample

The sample was prepared by adding KOH solution to an aqueous solution of H_2WO_4 .

Color

Colorless

Structure

Monoclinic, $C2/m$ (12), $Z = 4$. The structure was determined by Koster et al. (1969).

NBS lattice constants:

$$\begin{aligned} a &= 12.383(1) \text{ \AA} \\ b &= 6.1194(8) \\ c &= 7.5526(9) \\ \beta &= 115.95(1)^\circ \end{aligned}$$

Density

(calculated) 4.208 g/cm^3

Polymorphism

K_2WO_4 undergoes a transition at 370°C [Schmitz-Dumont and Weeg, 1951]

Additional patterns

1. PDF card 19-1004 [Gelsing et al., 1965]
2. PDF card 21-703 [Hatterer et al., 1968]
3. Kools et al. [1970]

References

- Gelsing, R. J. H., Stein, H. N., and Stevels, J.M. (1965). *Rec. Trav. Chim.* **84**, 1452.
- Hatterer, A., Kessler, H., and Ringenbach, C. (1968). *Compt. Rend. Paris* **266C**, 328.
- Kools, F. X. N. M., Koster, A. S., and Rieck, G.D. (1970). *Acta Cryst.* **B26**, 1974.
- Koster, A.S., Kools, F. X. N. M., and Rieck, G.D. (1969). *Acta Cryst.* **B25**, 1704.
- Schmitz-Dumont, O. and Weeg, A. (1951). *Z. Anorg. Chem.* **265**, 139.

Internal standard W, $a = 3.16516 \text{ \AA}$ $CuK\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
6.80	8	001	13.00
5.70	50	201	15.52
5.566	30	200	15.91
5.365	30	110	16.51
4.719	90	111	18.79
3.834	45	111	23.18
3.708	25	202	23.98
3.601	25	201	24.70
3.397	85	002	26.21
3.173	100	310	28.10
3.092	19	401	28.85
3.059	60	020	29.17
2.928	60	312	30.51
2.848	4	402	31.38
2.784	14	400	32.12
2.696	9	221	33.20
2.683	7	220	33.37
2.630	6	112	34.06
2.359	6	222	38.11
2.332	13	221	38.57
2.324	9	403	38.71
2.293	17	313	39.26
2.273	45	022	39.62
2.253	12	401	39.98
2.240	11	512	40.22
2.176	5	421	41.46
2.092	3	510	43.22
2.048	11	602	44.18
2.030	4	601	44.59
2.006	2	130	45.17
1.978	25	312	45.83
1.967	10	131	46.10
1.944	5	113, 223	46.69
1.899	6	603	47.85
1.885	5	131	48.25
1.868	4	204	48.71
1.855	11	600, 404	49.07
1.849	12	423	49.23
1.835	2	203	49.63
1.814	8	421	50.26
1.804	16	314	50.56
1.788	14	330	51.04
1.740	9	332	52.55
1.706	11	514	53.69
1.702	13	622	53.82

Potassium tungsten oxide, K_2WO_4 – continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.6984	10	$\bar{7}12,004$	53.94
1.6671	3	$\bar{6}04$	55.04
1.6607	6	$\bar{7}11$	55.27
1.6351	3	$\bar{7}13$	56.21
1.6133	3	$\bar{6}23$	57.04
1.5946	6	$\bar{2}24$	57.77
1.5866	9	$620,\bar{4}24$	58.09
1.5742	6	$223,\bar{3}33$	58.59
1.5559	4	$\bar{5}32$	59.35
1.5514	4	422	59.54
1.5474	3	$\bar{8}02$	59.71
1.5293	7	$040,114$	60.49
1.5043	2	530	61.60
1.4846	5	024	62.51
1.4649	8	$\bar{6}24$	63.45
1.4620	11	$\bar{3}15$	63.59
1.4601	8	332	63.68
1.3854	6	$\bar{3}34,531$	67.56
1.3803	5	$822,711$	67.84
1.3715	2	441	68.34
1.3384	5	$\bar{9}12,\bar{7}15$	70.27
1.3337	4	913	70.56
1.3075	4	$314,\bar{2}43$	72.19
1.3000	3	$\bar{6}25$	72.67

Sodium bromide chloride, $\text{NaBr}_{.33}\text{Cl}_{.67}$

Sample

The sample was prepared by melting a 1:2 mixture of NaBr and NaCl. After grinding it was annealed for 18 hours at 600 °C in a sealed glass tube.

Color

Colorless

Optical data

Isotropic, $N=1.577$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z=4$. There is a complete solid solution between NaBr and NaCl [Gromakov and Gromakova, 1955].

NBS lattice constant:
 $a = 5.7614(2)\text{\AA}$

Density

(calculated) 2.54 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 4.2$

Reference

Gromakov, S.P. and Gromakova, L.M. (1955). Zh.Fiz. Khim. 29, 746.

Internal standard W, $a = 3.16516 \text{\AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}$; temp. 25 °C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
3.329	30	111	26.76
2.882	100	200	31.00
2.037	45	220	44.43
1.7373	6	311	52.64
1.6632	11	222	55.18
1.4401	5	400	64.67
1.3216	2	331	71.30
1.2883	9	420	73.44
1.1761	5	422	81.83
1.1089	1	511	88.00
1.0185	1	440	98.28
0.9739	<1	531	104.54
.9603	1	600	106.67
.9108	1	620	115.49
.8686	1	622	124.95
.8317	<1	444	135.68
.8067	<1	711	145.43
.7990	<1	640	149.18

Sodium bromide chloride, $\text{NaBr}_{.67}\text{Cl}_{.33}$

Sample

The sample was prepared by melting a 2:1 mixture of NaBr and NaCl. After grinding it was annealed for 18 hours at 600 °C in a sealed glass tube.

Color

Colorless

Optical data

Isotropic, $N = 1.610$

Structure

Cubic, $\text{Fm}\bar{3}\text{m}$ (225), $Z=4$. There is a complete solid solution series between NaBr and NaCl [Gromakov and Gromakova, 1955].

NBS lattice constant:

$$a = 5.8676(2) \text{ \AA}$$

Density

(calculated) 2.87 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 5.5$

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
3.387	60	111	26.29
2.933	100	200	30.45
2.0742	60	220	43.60
1.7692	12	311	51.62
1.6944	18	222	54.08
1.4669	6	400	63.35
1.3463	4	331	69.80
1.3121	15	420	71.90
1.1977	9	422	80.05
1.1292	3	511	86.02
1.0375	2	440	95.88
.9918	2	531	101.91
.9780	4	600	103.93
.9277	3	620	112.26
.8949	<1	533	118.80
.8846	2	622	121.09
.8216	<1	711	139.28
.8136	1	640	142.42

References

Gromakov, S. P. and Gromakova, L. M. (1955). Zh. Fiz. Khim. 29, 746.

Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$

Sample

The sample was prepared by melting together equal molar amounts of Na_2CO_3 and Na_2SO_4 .

Major impurities

~ .05% Ag, Al, Ca, K and Si.

Color

Colorless

Optical data

Uniaxial (-), $N \approx 1.45$

Structure

Hexagonal, $P\bar{3}m1$ (164), $Z=1$, isostructural with Na_2SO_4 , form I, and with $\alpha\text{-Na}_2\text{CO}_3$. A continuous isomorphous series exists in all proportions from zero to 75 mol. percent Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

$a = 5.2284(5) \text{ \AA}$

$c = 6.8808(8)$

Density

(calculated) 2.528 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 1.1$

Polymorphism

The 1:1 composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
4.528	7	100	19.59
3.783	60	101	23.50
3.440	45	002	25.88
2.741	100	102	32.64
2.614	70	110	34.28
2.263	2	200	39.80
2.150	14	201	41.98
1.891	35	202	48.07
1.720	8	004	53.20
1.710	4	210	53.53
1.611	1	203	57.14
1.5322	9	212	60.36
1.5094	6	300	61.37
1.4366	8	114	64.85
1.3825	1	302	67.72
1.3722	1	213	68.30
1.3166	1	105	71.61
1.3073	6	220	72.20
1.2218	5	222	78.17
1.1796	3	312	81.54
1.1467	1	006	84.40
1.1347	3	304	85.51
1.1119	1	106	87.70
1.1016	1	313	88.73
1.0753	2	402	91.51
1.0407	2	224	95.49

References

- Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.
 Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
 Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

Sodium carbonate sulfate (burkeite), $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$

Sample

The sample was precipitated by mixing boiling aqueous solutions of Na_2CO_3 and Na_2SO_4 in a molar ratio of 1:2. Chemical analysis of the precipitate indicated a ratio of 1:2.0.

Color

Colorless

Structure

Orthorhombic, $Z=4/3$. Ramsdell [1942] reported a cell with the a and b parameters tripled. No evidence was seen here for an enlarged cell. This phase occurs over a range of solid solution [Caspari, 1924] [Schroeder et al., 1936]. Khlapova and Burovaya [1957] reported that this phase ("rhombic" burkeite) contained essential H_2O . However the weight loss found at NBS between 350 and 700 °C was only 0.32% after the material had been transformed to the hexagonal form of the $\alpha\text{-Na}_2\text{SO}_4$ type.

NBS lattice constants:
 $a = 7.055(2)\text{Å}$
 $b = 9.215(2)$
 $c = 5.167(1)$

Density

(calculated) 2.571 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 0.7$

Polymorphism

In studies of the system $\text{Na}_2\text{CO}_3\text{-Na}_2\text{SO}_4$ Khlapova and Burovaya [1957] and Khlapova and Kovaleva [1963] found three hexagonal polymorphs of the 1:2 composition, not including this one which they considered a hydrate. Transitions were reported to occur at 400 and 575 °C.

Additional patterns

1. PDF card 2-840 [Michigan Alkali Co. Wyandotte Michigan].
2. Ramsdell [1939].

References

- Caspari, W. A. (1924). J. Chem. Soc. 125, 2381.
 Khlapova, A.N. and Burovaya, E.E. (1957). Russ. J. Inorg. Chem. (English Transl.) 2, No.8, 249.
 Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
 Ramsdell, L.S. (1939). Am. Mineralogist 24, 109.
 Ramsdell, L.S. (1942). Am. Mineralogist 27, 230.

Internal standard Ag, $a = 4.08641\text{ Å}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056\text{ Å}$; temp. 25 °C			
$d\text{ (Å)}$	I	hkl	$2\theta(^{\circ})$
9.215	8	010	9.59
4.607	5	020	19.25
4.507	17	011	19.68
4.172	4	101	21.28
3.854	40	120	23.06
3.795	75	111	23.42
3.526	80	200	25.24
3.439	19	021	25.89
3.307	3	210	26.99
3.072	17	030	29.04
2.801	100	220	31.93
2.777	55	211	32.21
2.640	75	031	33.93
2.583	75	002	34.70
2.488	5	012	36.07
2.345	6	112	38.35
2.305	11	040	39.05
2.279	4	310	39.51
2.191	3	140	41.17
2.147	14	122	42.04
2.142	11	301	42.15
2.105	6	041	42.94
1.978	12	032	45.84
1.929	30	240	47.07
1.904	25	132	47.74
1.898	30	222	47.88
1.784	2	150	51.17
1.764	17	400	51.79
1.735	8	051	52.71
1.722	3	003	53.15
1.673	2	103	54.83
1.645	3	113, 340+	55.85
1.635	4	250	56.20
1.627	4	322	56.53
1.614	4	023	57.00
1.557	5	251	59.30
1.548	6	203	59.67
1.545	5	242	59.82
1.536	6	060	60.20
1.526	5	213	60.64
1.503	6	033	61.67

Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$

Sample

The sample was prepared by melting a 1:2 molar mixture of Na_2CO_3 and Na_2SO_4 . The sample was somewhat hygroscopic.

Color

Colorless

Structure

Hexagonal, $P\bar{3}m1$ (164), $Z=2$, isostructural with Na_2SO_4 , form I, and with $\alpha\text{-Na}_2\text{CO}_3$. A continuous series of isomorphous phases occurs in all proportions from zero to 75 mol. percent of Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

$$a = 5.2624(4) \text{ \AA}$$

$$c = 7.0236(7)$$

Density

(calculated) 2.563 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.1$$

Polymorphism

This composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

References

- Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.
 Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
 Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
4.558	10	100	19.46
3.824	85	101	23.24
3.515	50	002	25.32
2.783	100	102	32.14
2.631	80	110	34.05
2.279	4	200	39.51
2.167	11	201	41.65
2.106	1	112	42.90
1.912	40	202	47.51
1.755	10	004	52.06
1.7227	3	210	53.12
1.6332	2	203	56.28
1.5471	11	212	59.72
1.5190	7	300	60.94
1.4848	1	301	62.50
1.4603	10	114	63.67
1.3949	2	302	67.04
1.3876	2	213	67.44
1.3424	1	105	70.03
1.3154	5	220	71.69
1.2639	1	310	75.10
1.2439	1	311	76.52
1.2318	2	222	77.41
1.1892	3	312	80.74
1.1706	1	006	82.30
1.1488	4	304	84.21
1.1337	2	106	85.60
1.1121	2	313	87.68
1.0887	<1	215	90.07
1.0837	2	402	90.60
1.0529	2	224	94.04
1.0409	<1	206	95.47

Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$

Sample

The sample was prepared by melting Na_2CO_3 and Na_2SO_4 together in a 2:1 molar ratio.

Major impurities

~ .05% Ca

Color

Colorless

Structure

Hexagonal, $\bar{P}3m1$ (164), $Z=2$, isostructural with Na_2SO_4 , form I, and with $\alpha\text{-Na}_2\text{CO}_3$. A continuous isomorphous series exists in all proportions from zero to 75 mol. percent Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

$a = 5.2034(5)\text{\AA}$

$c = 6.683(1)$

Density

(calculated) 2.501 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 0.7$

Polymorphism

This composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

Internal standard Ag, $a = 4.08641\text{\AA}$

$\text{CuK}\alpha_1$, $\lambda = 1.54056\text{\AA}$; temp. 25°C

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$
4.505	4	100	19.69
3.739	45	101	23.78
3.341	55	002	26.66
2.684	100	102	33.35
2.603	75	110	34.43
2.253	2	200	39.99
2.135	25	201	42.29
1.868	35	202	48.72
1.7034	5	210	53.77
1.6707	6	004	54.91
1.6508	2	211	55.63
1.5836	2	203	58.21
1.5181	6	212	60.98
1.5019	6	300	61.71
1.4655	1	301	63.42
1.4062	4	114	66.43
1.3527	1	213	69.42
1.3008	5	220	72.62
1.2814	<1	105	73.90
1.2453	1	303	76.42
1.2125	3	222	78.88
1.1706	3	312	82.30

References

- Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.
- Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
- Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$

Sample

The sample was prepared by melting an equimolar mixture of Na_2SO_4 and Na_2CrO_4 . This material was then annealed for 18 hours at 600 °C, followed by 350 °C for 2 hours in a stream of oxygen.

Color

Brilliant greenish yellow

Structure

Orthorhombic, Amam (63), $Z=2$, isostructural with Na_2CrO_4 and Na_2SO_4 (III) [Fischmeister, 1954]. The structure of Na_2CrO_4 was determined by Miller [1936], and the space group was corrected by Niggli [1954]. Na_2CrO_4 and Na_2SO_4 (III) form a complete isomorphous series [Fischmeister, 1954].

NBS lattice constants:

$a = 7.055(2) \text{ \AA}$

$b = 9.115(2)$

$c = 5.744(2)$

Density

(calculated) 2.733 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 0.8$

Major impurities

~ .05% Ag and Al

References

Fischmeister, H. (1954). Acta Cryst. 7, 776.
Miller, J.J. (1936). Z. Krist. 94, 131.
Niggli, A. (1954). Acta Cryst. 7, 776.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
4.857	15	011	18.25
4.555	3	020	19.47
4.003	50	111	22.19
3.831	45	120	23.20
3.527	55	200	25.23
2.869	75	002	31.15
2.855	100	211	31.30
2.687	60	031	33.32
2.511	2	131	35.73
2.430	20	022	36.96
2.280	3	040	39.49
2.168	2	140	41.62
2.135	6	231	42.29
2.116	3	311	42.70
2.089	7	320	43.28
2.000	16	222	45.30
1.915	9	240	47.44
1.811	2	113	50.34
1.770	10	331	51.60
1.764	20	400	51.79
1.686	1	151	54.31
1.656	4	213	55.45
1.619	8	033	56.81
1.5926	10	242	57.85
1.5585	2	251	59.24
1.5032	2	402	61.65
1.4742	10	431	63.00

Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$

Sample

The sample was made by reacting a saturated solution of sodium hydrogen carbonate with a suspension of basic magnesium carbonate.

Color

Colorless

Optical data

Uniaxial (-), $N_e = 1.450$, $N_o = 1.605$ [Pabst, 1973].

Structure

Hexagonal, $\bar{R}3$ (148), $Z = 3$ [Pabst, 1973]. Eitel and Skalijs [1929] previously reported $\bar{P}3$ (147) as the space group.

NBS lattice constants:

$a = 4.9423(2) \text{ \AA}$

$c = 16.396(1)$

Density

(calculated) 2.792 g/cm^3

Reference intensity

I/I_{corundum} 1.8

Additional patterns

1. PDF card 4-737 [Wyandotte Chem. Co., Wyandotte, Michigan]

References

Eitel, W. and Skalijs, W. (1929). Z. anorg. u. allgem. Chem. 183, 263.
Pabst, A. (1973). Am. Mineralogist 58, 211.

Internal standard W, $a = 3.16516 \text{ \AA}$

$\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C

$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
5.48	<1	003	16.17
3.794	16	012	23.43
2.731	25	006	32.77
2.602	100	015	34.44
2.469	25	110	36.36
2.251	20	113	40.03
2.121	2	021	42.58
2.0710	18	202	43.67
1.8975	20	024	47.90
1.8486	2	018	49.25
1.8333	9	116	49.69
1.7925	9	205	50.90
1.6099	8	211	57.17
1.5873	2	122	58.06
1.5311	11	1-0-10	60.41
1.5048	1	214	61.58
1.4803	1	208	62.71
1.4663	4	119	63.38
1.4505	6	125	64.15
1.4264	5	300	65.37
1.3802	<1	303	67.85
1.3665	1	0-0-12	68.62
1.3310	1	217	70.72
1.3016	<1	0-2-10	72.57
1.2695	1	128	74.71
1.2355	4	220	77.14
1.2232	<1	2-0-11	78.06
1.1957	<1	1-1-12	80.21
1.1841	1	131	81.16
1.1749	<1	312	81.93
1.1516	3	2-1-10	83.96
1.1297	<1	0-1-14	85.98
1.1233	<1	309	86.59
1.1163	4	315	87.27
1.0962	<1	1-2-11	89.29
1.0930	1	0-0-15	89.62
1.0865	<1	0-2-13	90.30
1.0588	<1	137	93.35
1.0353	<1	404	96.15
1.0271	<1	2-0-14, 318	97.18
1.0227	<1	229	97.74
1.0172	1	045	98.44
0.9996	<1	1-1-15	100.82
.9947	<1	2-1-13	101.50
.9750	<1	232	104.38
.9615	1	1-3-10	106.47
.9550	<1	324	107.53
.9488	<1	1-2-14, 048	108.55
.9406	1	235	109.95
.9340	1	410	111.12

Sodium sulfate, Na₂SO₄

Sample

The sample was prepared by heating Na₂SO₄ at 700 °C for one hour. The sample changes to Na₂SO₄, form V, if exposed to moist air.

Color

Colorless

Structure

Orthorhombic, Amam (63), Z=4, isostructural with Na₂CrO₄ [Frevel, 1940]. The structure of Na₂CrO₄ was determined by Miller [1936]. The space group was corrected by Niggli [1954].

NBS lattice constants:
a = 6.9666(9) Å
b = 8.9511(9)
c = 5.6109(6)

Density

(calculated) 2.696 g/cm³

Reference intensity

I/I_{corundum} = 1.8

Polymorphism

The polymorphism of Na₂SO₄ is complex and not completely resolved. The form reported here is stable at room temperature and has been referred to as Na₂SO₄, form III; Na₂SO₄, form I, is hexagonal and is stable above 250°C. [Kracek and Ksanda, 1930]. Khlapova [1956] reported a form (δ), stable between 600°C. and the melting point (900°C.). Khlapova and Burovaya [1957] discussed the phase of Na₂SO₄ known as form V and as the mineral thenardite. They considered it to be a hydrate.

Additional patterns

1. PDF card 8-31 [Fischmeister, 1954]
2. Das Gupta [1954]

References

- Das Gupta, D. R. (1954). Acta Cryst. 7, 275.
Fischmeister, H. (1954). Acta Cryst. 7, 776.
Frevel, L.K. (1940). J. Chem. Phys. 8, 290.
Khlapova, A.N. (1956). Russ. J. Inorg. Chem. (English Transl.) 1, No. 11, 132.
Khlapova, A.N. and Burovaya, E.E. (1957). Russ. J. Inorg. Chem. (English Transl.) 2, No.8, 249.
Kracek, F. C. and Ksanda, C. J. (1930). J. Phys. Chem. 34, 1741.
Miller, J.J. (1936). Z. Krist. 94, 131.
Niggli, A. (1954). Acta Cryst. 7, 776.

Internal standard Ag, a = 4.08641 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C			
d (Å)	I	hkl	2θ (°)
4.759	9	011	18.63
4.476	4	020	19.82
3.929	35	111	22.61
3.768	30	120	23.59
3.485	25	200	25.54
2.809	100	211,002	31.83
2.636	45	031	33.98
2.465	2	131	36.42
2.377	20	022	37.82
2.238	4	040	40.26
2.184	2	202	41.31
2.131	6	140	42.39
2.101	6	231	43.01
2.086	7	311	43.33
2.062	5	320	43.87
1.963	18	222	46.20
1.883	9	240	48.29
1.831	1	013	49.76
1.771	1	113	51.56
1.7496	13	042	52.24
1.7419	18	331,400	52.49
1.6964	2	142	54.01
1.6229	3	420	56.67
1.6206	4	213	56.76
1.6115	3	340	57.11
1.5845	9	033	58.17
1.5633	10	242	59.04
1.5320	3	251	60.37
1.4919	1	060	62.17
1.4799	2	402	62.73
1.4528	9	431	64.04
1.4425	2	233	64.55
1.4028	4	004	66.61
1.3748	3	351,440	68.15
1.3370	1	511	70.36
1.3302	2	520	70.77
1.3168	3	062	71.60
1.3144	2	124	71.75
1.2941	3	162	73.06
1.2714	2	153	74.58
1.2494	1	224	76.12
1.2317	2	262,531	77.42

Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by heating $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ at 60 - 70 °C for several hours under vacuum.

Color

Colorless

Structure

Monoclinic, Cc (9) or C2/c (15), Z=4. The structure was determined by Jensen [1942].

NBS lattice constant:

$$a = 11.688(1) \text{ \AA}$$

$$b = 6.4048(5)$$

$$c = 6.6957(6)$$

$$\beta = 105.54(1)^\circ$$

Density

(calculated) 2.676 g/cm³

Reference intensity

I/I_{corundum} 1.0

Additional patterns

1. PDF card 3-500 [Jensen, 1942].

References

Jensen, A.T. (1942). Kgl. Danske Videnskab. Selskab Mat. Fys. Medd. 20, Nr.5.

Internal standard W, $a = 3.16516 \text{ \AA}$

$\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25 °C

$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.63	60	200	15.74
4.523	75	111	19.61
3.964	35	111	22.41
3.238	35	310	27.52
3.229	30	002	27.60
3.206	100	311, 020	27.80
2.966	4	112	30.10
2.871	20	021	31.13
2.816	2	400	31.75
2.784	45	220	32.12
2.690	30	221	33.28
2.659	75	311	33.68
2.645	40	112	33.86
2.608	20	312	34.36
2.523	35	202	35.55
2.475	30	402	36.27
2.442	14	221	36.78
2.272	30	022	39.63
2.261	35	222	39.84
2.189	13	511	41.20
2.140	1	421	42.19
2.125	2	510	42.51
2.114	35	420	42.74
2.101	40	113	43.01
2.025	30	512, 131	44.71
2.020	30	313	44.83
1.982	9	222	45.74
1.966	30	131	46.13
1.959	5	422	46.31
1.922	6	113	47.25
1.900	2	421	47.84
1.8816	20	511	48.33
1.8765	18	600	48.47
1.8522	13	602	49.15
1.7481	2	513	52.29
1.7236	2	331	53.09
1.7096	1	332	53.56
1.6866	2	423	54.35
1.6640	7	621	55.15
1.6253	8	422	56.58
1.6190	7	620	56.82
1.6151	6	711	56.97
1.6066	6	114	57.30
1.6020	6	223, 040	57.48
1.5979	10	314, 512	57.64
1.5740	6	712, 531	58.60
1.5599	3	710	59.18
1.5401	8	133, 240	60.02
1.5240	7	332, 241	60.72
1.5072	4	333	61.47

Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	2θ (°)
1.4833	6	$\bar{2}24$	62.57
1.4765	4	$\bar{5}14$	62.89
1.4651	8	133	63.44
1.4609	6	602	63.64
1.4554	4	$\bar{7}13$	63.91
1.4507	6	204	64.14
1.4401	5	024	64.67
1.4342	6	042, $\bar{7}11$	64.97
1.4309	10	$\bar{2}42$	65.14
1.4270	5	$\bar{6}04$	65.34
1.4073	5	800	66.37
1.3916	7	440	67.22
1.3836	9	$\bar{5}33$	67.66
1.3502	8	$\bar{5}13$	69.57
1.3443	4	$\bar{4}42$	69.92
1.3289	8	622	70.85
1.3252	5	441	71.08
1.3208	9	333	71.35
1.3149	5	$\bar{7}31$	71.72
1.3127	3	$\bar{8}22$	71.86
1.3034	6	$\bar{7}14, \bar{6}24$	72.45
1.2948	3	$\bar{1}15$	73.01
1.2886	3	820	73.42
1.2726	4	150	74.50
1.2691	5	$\bar{9}11$	74.74
1.2558	4	$\bar{1}51$	75.67
1.2523	5	$\bar{5}15$	75.92
1.2488	5	134, $\bar{8}23$	76.17
1.2416	3	151	76.69
1.2280	2	910	77.70
1.2244	2	$\bar{7}33$	77.97
1.2208	6	442	78.24
1.2112	8	731, $\bar{6}42$	78.98

Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl}_{.65}(\text{OH})_{.35}(\text{PO}_4)_3$

Sample

The sample was prepared by adding a Na_3PO_4 solution to a saturated solution of SrCl_2 . After boiling, the precipitate was filtered, washed, dried, and heated to 1100 °C for one half hour. Analysis showed 3.07 percent chlorine.

Color

Colorless

Structure

Hexagonal, $\text{P6}_3/\text{m}$ (176), $Z=2$, isostructural with calcium hydroxyapatite, $\text{Ca}_5\text{OH}(\text{PO}_4)_3$; its structure was determined by Posner et al. [1958]. There is a complete solid solution between $\text{Sr}_5\text{OH}(\text{PO}_4)_3$ and $\text{Sr}_5\text{Cl}(\text{PO}_4)_3$. However, the structure of $\text{Ca}_5\text{Cl}(\text{PO}_4)_3$ was determined by Mackie et al. [1972] and found to be monoclinic, pseudo-hexagonal. The data here gave no indication of a departure from hexagonal.

NBS lattice constants:

$a = 9.847(1)\text{\AA}$
 $c = 7.219(1)$

Density

(calculated) 4.119 g/cm^3

Reference intensity

I/I_{corundum} 3.0

Additional patterns

1. PDF 16-666 [General Electric Co. Ltd., Wembley England - for $\text{Sr}_5\text{Cl}(\text{PO}_4)_3$].

References

Mackie, P.E., Elliott, J.C., and Young, R.A. (1972) Acta Cryst. B28, 1840.
Posner, A.S., Perloff, A., and Diorio, A.F. (1958) Acta Cryst. 11, 308.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
8.51	2	100	10.39
5.50	2	101	16.10
4.93	3	110	17.98
4.263	13	200	20.82
4.070	9	111	21.82
3.609	13	002	24.65
3.325	11	102	26.79
3.225	20	210	27.64
2.942	95	211	30.36
2.910	100	112	30.70
2.842	55	300	31.45
2.755	3	202	32.47

$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
2.645	1	301	33.86
2.464	1	220	36.44
2.404	2	212	37.37
2.365	9	310	38.02
2.247	2	311	40.10
2.232	6	302	40.37
2.162	9	113	41.75
2.132	2	400	42.35
2.096	2	203	43.12
2.033	35	222	44.52
1.978	11	312	45.83
1.956	4	329	46.39
1.928	25	213	47.10
1.888	15	321	48.16
1.861	15	410	48.90
1.835	14	402,303	49.63
1.804	9	004	50.54
1.721	<1	223, 322	53.18
1.695	1	114	54.07
1.687	2	313	54.32
1.662	1	204	55.22
1.655	4	412	55.49
1.640	1	330	56.02
1.6120	3	420	57.09
1.6004	2	331	57.54
1.5745	5	214	58.58
1.5417	3	502	59.95
1.5318	1	510	60.38
1.5236	10	304	60.74
1.5186	10	323	60.96
1.4975	7	511	61.91
1.4943	7	332	62.06
1.4725	1	413,422	63.08
1.4346	<1	314	64.95
1.4101	1	512	66.22
1.3775	2	404	68.00
1.3658	1	520	68.66
1.3563	1	333	69.21
1.3418	2	521	70.07
1.3389	3	423	70.24
1.3261	2	324	71.02
1.3224	3	602	71.25
1.3178	4	215	71.54
1.3067	2	432	72.24
1.2954	9	414	72.97
1.2774	7	522	74.17
1.2310	3	440	77.47
1.2142	1	334	78.75
1.2115	1	433	78.96
1.2021	3	424	79.70
1.1875	1	523	80.88
1.1680	4	514	82.52
1.1618	2	325	83.06
1.1543	2	532	83.72

Strontium oxide hydrate, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$

Sample

A solution of SrCl_2 was treated with a slight excess of three percent H_2O_2 and stirred. Dilute NH_4OH solution was added and the precipitate was dried at room temperature. Since the crystals were very thin platelets, orientation may have affected intensity measurements.

Color

Colorless

Structure

Tetragonal, $P4/mcc$ (124), $Z=2$. The structure was determined by Vannerberg [1959].

NBS lattice constants:

$$a = 6.3432(5) \text{ \AA}$$

$$c = 11.197(1)$$

Density

(calculated) 1.944 g/cm^3

Additional patterns

1. PDF card 12-521 [Vannerberg, 1959].
2. PDF card 2-1245 [Natta, 1932].

References

Natta, G. (1932). Gazz. Chim. Ital. 62, 444.
Vannerberg, N-G. (1959). Arkiv Kemi 14, 17.

Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1$, $\lambda = 1.54056 \text{ \AA}$; temp. 25°C			
$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
6.36	2	100	13.92
5.59	100	002	15.85
4.49	2	110	19.74
4.197	7	102	21.15
3.496	9	112	25.46
2.798	10	004	31.96
2.759	4	202	32.42
2.750	4	211	32.53
2.560	9	104	35.02
2.530	2	212	35.45
2.377	11	114	37.82
2.258	2	213	39.89
2.242	1	220	40.18
2.098	5	204	43.09
2.081	1	222	43.45
2.007	2	310	45.14
1.992	5	214	45.50

$d (\text{\AA})$	I	hkl	$2\theta (^\circ)$
1.979	<1	302	45.81
1.889	2	312	48.14
1.866	1	006	48.75
1.791	8	106	50.95
1.758	1	320,215	51.97
1.723	1	116	53.10
1.687	<1	304	54.32
1.678	<1	322	54.64
1.608	<1	206	57.23
1.559	4	216	59.20
1.526	<1	402	60.64
1.490	<1	324	62.24
1.444	<1	332	64.48
1.434	<1	226	64.94
1.418	<1	420	65.81
1.399	4	008,306	66.79
1.394	1	217	67.11
1.379	1	404	67.90
1.374	1	422	68.18
1.367	4	108,316	68.62
1.348	<1	414	69.67
1.336	<1	118	70.41
1.319	<1	334	71.47
1.280	<1	208,326	73.98
1.255	1	218	75.71
1.187	1	228,416	80.93
1.167	1	308,336	82.59
1.155	<1	434	83.63
1.153	<1	522	83.85
1.148	1	318	84.30
1.139	<1	219	85.09
1.120	<1	0-0-10	86.91
1.103	1	1-0-10	88.61
1.095	1	328	89.41
1.086	<1	1-1-10	90.33
1.056	<1	2-0-10	93.67
1.0414	1	2-1-10	95.40
1.0352	1	418,516	96.16
1.0014	<1	2-2-10	100.56
.9960	1	428,526	101.31
.9891	<1	604	102.30
.9774	<1	3-1-10,614	104.01
.9754	<1	542	104.31
.9580	<1	2-1-11	107.04
.9446	<1	3-2-10	109.27
.9398	<1	438,536	110.10
.9231	<1	1-0-12	113.12
.9133	<1	1-1-12	115.00
.9053	<1	4-1-10	116.60
.9012	<1	528	117.44
.8952	<1	2-0-12	118.73
.8862	<1	2-1-12	120.72

Strontium phosphate, alpha $\text{Sr}_2\text{P}_2\text{O}_7$

Sample

The sample was prepared by adding dilute NH_4OH to a hot concentrated aqueous solution of SrCl_2 and Na_3PO_4 . The precipitate was filtered, washed with alcohol, and heated to 1200 °C for ten minutes.

Major impurities

~ .05% Al, Ba, Ca, Mg, Co, and V.

Color

Colorless

Structure

Orthorhombic, $Z=4$, isostructural with $\alpha\text{-Ca}_2\text{P}_2\text{O}_7$ [Wanmaker and ter Vrugt, 1967], [Ranby et al. 1955].

NBS lattice constants:

a = 8.917(2) Å

b = 13.169(2)

c = 5.400(1)

Density

(calculated) 3.657 g/cm³

Reference intensity

I/I_{corundum} = 2.3

Polymorphism

The alpha form is stable above 750 °C [Ranby et al., 1955]. Below 750 °C the alpha form very slowly changes to the beta form. The beta form is represented by PDF card 13-194 [Hoffman and Mooney, 1960].

Additional patterns

1. PDF card 12-362 [Ropp et al., 1959]

Internal standard Ag, $a = 4.08641$ Å

$\text{CuK}\alpha_1$ $\lambda = 1.54056$ Å; temp. 25 °C

d (Å)	I	hkl	2θ (°)
7.40	35	110	11.95
6.60	13	020	13.41
5.30	3	120	16.70
5.01	3	011	17.70
4.462	11	200	19.88
3.940	9	130	22.55
3.694	4	220	24.07
3.439	85	201	25.89
3.406	100	031	26.14
3.327	35	211	26.77
3.291	4	040	27.07
3.182	15	131	28.02
3.128	25	230	28.51
3.087	2	140	28.90
3.048	7	221	29.28
2.900	20	310	30.81
2.700	45	002	33.15
2.680	25	141	33.41
2.648	2	240,012	33.82
2.554	14	311	35.11
2.525	11	150	35.52
2.422	7	321	37.09
2.406	10	122	37.35
2.377	2	241	37.81
2.310	5	202	38.95
2.274	2	212	39.60
2.239	6	331	40.25
2.230	9	400	40.42
2.195	30	060	41.08
2.132	6	160	42.36
2.090	1	251	43.25
2.044	65	232	44.27
1.987	7	430	45.61
1.982	8	161	45.73
1.976	9	312	45.88
1.966	11	421	46.13
1.913	2	322	47.49
1.891	6	242	48.08
1.866	17	431	48.76
1.850	30	261	49.21
1.776	3	071	51.40
1.747	4	441	52.34
1.742	3	171	52.48
1.722	2	520	53.15
1.703	8	062,450	53.79
1.680	6	511	54.59
1.669	12	203	54.97
1.665	13	033	55.10
1.656	4	213	55.44
1.651	3	271	55.62

Strontium phosphate, alpha $\text{Sr}_2\text{P}_2\text{O}_7$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.6402	2	521	56.02
1.6370	3	133	56.14
1.6180	<1	223	56.86
1.6009	3	432	57.52
1.5903	7	370	57.94
1.5643	4	460	59.00
1.5554	3	143	59.37
1.5297	3	313	60.47
1.5249	2	371	60.68
1.5026	3	461	61.68

References

- Hoffman, C.W.W. and Mooney, R.W. (1960). J. Electrochem. Soc. 107, 8541.
- Ranby, P.W., Mash, D.H., and Henderson, S.T. (1955). Brit. J. Appl. Phys. 6, Supplement 4 S18.
- Ropp, R.C., Aia, M.A., Hoffman, C.W.W., Veleker, T.J., and Mooney, R.W. (1959). Anal. Chem. 31, 1163.
- Wanmaker, W.L. and ter Vrugt, J.W. (1967). Philips Res. Rep. 22, 355.

Strontium phosphate, α $\text{Sr}_3(\text{PO}_4)_2$

Sample

The sample was prepared by heating a 3:2 molar mixture of SrCO_3 and $(\text{NH}_4)_2\text{HPO}_4$ at 700°C , grinding, and reheating at 1200°C for 15 minutes.

Color

Colorless

Structure

Hexagonal, $R\bar{3}m$ (166), $Z = 3$, isostructural with $\text{Ba}_3(\text{PO}_4)_2$. The structure was determined by Zachariasen [1948].

NBS lattice constants:

$$a = 5.3871(2) \text{ \AA}$$

$$c = 19.780(1)$$

Density

(calculated) 4.537 g/cm^3

Reference intensity

I/I_{corundum} 4.4

Polymorphism

α - $\text{Sr}_3(\text{PO}_4)_2$ undergoes a readily reversible, polymorphic inversion at 1305°C to β - $\text{Sr}_3(\text{PO}_4)_2$ [Sarver et al., 1961].

Additional patterns

1. PDF card 14-271 [Sarver et al., 1961].
2. Zachariasen [1948].
3. PDF card 2-744 is for $\text{Sr}_5\text{OH}(\text{PO}_4)_3$ and not $\text{Sr}_3(\text{PO}_4)_2$.

References

- Sarver, J. F., Hoffman, M. V., and Hummel, F. A. (1961). J. Electrochem. Soc. **108**, 1103.
Zachariasen, W. H. (1948). Acta Cryst. **1**, 263.

Internal standard W, $a = 3.16516 \text{ \AA}$

$\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C

d (Å)	I	hkl	2θ (°)
6.60	1	003	13.40
4.554	7	101	19.52
4.225	1	012	21.01
3.393	10	104	26.24
3.016	100	015	29.59
2.694	85	110	33.23
2.494	<1	113	35.98
2.418	<1	107	37.15
2.318	3	021	38.82
2.271	11	202	39.66
2.198	11	009	41.03
2.186	2	018	41.27
2.110	14	024	42.82
2.087	7	116	43.32
2.009	35	205	45.08
1.821	20	1·0·10	50.05
1.799	2	027	50.69
1.7565	2	211	52.02
1.7360	<1	122	52.68
1.7031	9	119	53.78
1.6607	1	214	55.27
1.6107	20	125	57.14
1.5547	12	300	59.40
1.5087	6	0·2·10	61.40
1.4960	1	217	61.98
1.4360	<1	128	64.88
1.4243	<1	2·0·11	65.48
1.4066	1	306,1·1·12	66.41
1.3521	3	0·1·14	69.46
1.3468	10	220	69.77
1.3162	12	2·1·10	71.64
1.2913	<1	131	73.24
1.2827	<1	312	73.81
1.2746	<1	0·2·13	74.36
1.2697	2	309	74.70
1.2517	1	134	75.96
1.2298	7	315	77.56
1.2087	1	2·0·14	79.18
1.1844	8	1·1·15	81.14
1.1643	<1	401	82.84
1.1583	<1	042	83.37
1.1484	3	229	84.25
1.1353	<1	404	85.45
1.1288	<1	0·1·17	86.06
1.1188	3	045	87.02
1.1026	2	1·2·14	88.63
1.0828	4	1·3·10	90.69
1.0461	<1	324	94.84
1.0333	5	235	96.40
1.0182	4	410	98.32

Strontium phosphate, alpha $\text{Sr}_3(\text{PO}_4)_2$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$
1.0161	3	1·0·19	98.59
1.0057	4	3·0·15	99.98
1.0049	2	4·0·10	100.09
0.9822	<1	238	103.30
.9784	<1	0·4·11	103.86
.9728	<1	416	104.71
.9711	<1	1·2·17	104.97
.9675	1	0·1·20	105.53
.9542	1	3·1·14	107.66
.9508	1	0·2·19	108.22
.9422	3	2·2·15	109.68
.9414	3	3·2·10	109.82
.9237	1	419	113.00
.9170	<1	054	114.29
.9105	<1	2·0·20	115.55
.9081	1	505	116.04
.8994	1	0·4·14	117.83
.8978	1	330	118.18
.8964	2	2·1·19	118.47
.8891	<1	1·1·21	120.07
.8828	<1	1·0·22	121.50
.8782	<1	422	122.59
.8680	<1	244	125.11
.8661	<1	336, 4·1·12	125.59
.8626	2	1·2·20	126.51
.8605	4	425	127.05
.8531	1	2·3·14	129.08
.8438	1	0·5·10	131.80

Sample

The sample used was an NBS Standard Reference Material (Number 17)
 moisture..... less than 0.01%
 ash..... less than 0.01%
 reducing substances... less than 0.02%

Color

Colorless

Optical data

Biaxial(-), $N_\alpha=1.540$, $N_\beta=1.558$, $N_\gamma=1.564$; 2V is medium

Structure

Monoclinic, $P2_1$ (4), $Z=2$, structure determined by Beevers et al. [1952], and refined by Brown and Levy [1963].

NBS lattice constants:
 $a = 10.868(2)\text{\AA}$
 $b = 8.710(1)$
 $c = 7.761(1)$
 $\beta = 102.97(1)^\circ$

Density

(calculated) 1.588 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 0.7$

Additional patterns

- PDF card 6-0142 [Palmer, Agriculture Res. Service, Albany, California]

References

- Brown, G.M. and Levy, H.A. (1963). Science **141**, 921.
 Beevers, C.A., McDonald, T.R.R., Robertson, J.H., and Stern, F. (1952). Acta Cryst. **5**, 689.

Internal standard W, $a = 3.16516\text{\AA}$ CuK α_1 $\lambda = 1.54056\text{\AA}$; temp. 25 °C			
$d\text{ (\AA)}$	I	hkl	$2\theta(^\circ)$
10.59	14	100	8.34
7.58	65	001	11.67
6.94	40	$\bar{1}01$	12.74
6.73	55	110	13.14
5.712	30	011	15.50
5.424	11	$\bar{1}11$	16.33
5.298	14	200	16.72
4.884	12	201	18.15
4.706	100	111	18.84
4.523	80	210	19.61
4.354	25	020	20.38
4.259	30	$\bar{2}11$	20.84
4.028	30	120	22.05
3.943	11	201	22.53
3.776	18	002,021	23.54
3.690	8	$\bar{1}21$	24.10
3.591	100	211	24.77
3.531	45	300	25.20
3.467	3	012, $\bar{2}02$	25.67
3.437	5	121	25.90
3.364	11	220	26.47
3.272	5	310	27.23
3.254	10	$\bar{2}21$	27.39
3.222	7	$\bar{2}12$	27.66
3.112	9	112	28.66
2.956	2	301	30.21
2.923	6	221	30.56
2.882	25	$\bar{1}22$	31.00
2.856	6	022	31.29
2.799	20	130,311+	31.95
2.777	4	$\bar{3}12$	32.21
2.742	10	320	32.63
2.711	4	$\bar{2}22,031$	33.01
2.677	10	$\bar{1}31$	33.44
2.661	4	212	33.65
2.648	2	400,122	33.82
2.586	5	$\bar{1}03$	34.66
2.574	4	131, $\bar{4}11$	34.82
2.545	3	230	35.24
2.521	5	003	35.58
2.504	6	$\bar{2}03$	35.83
2.496	7	$\bar{2}31$	35.95
2.479	9	$\bar{1}13$	36.20
2.444	5	321	36.74
2.430	6	$\bar{3}22$	36.96
2.406	9	$\bar{2}13$	37.34
2.349	40	222, $\bar{4}12$	38.28
2.339	16	401, $\bar{2}31+$	38.46
2.312	7	$\bar{3}03$	38.92
2.291	4	$\bar{4}21$	39.30

Sucrose, $C_{12}H_{22}O_{11}$ - continued

d (Å)	I	hkl	2θ (°)
2.258	14	113	39.89
2.253	11	312	39.98
2.234	10	$\bar{3}13$	40.33
2.189	5	132	41.20
2.171	5	$\bar{2}23, \bar{5}01$	41.57
2.133	1	140	42.34
2.101	2	203	43.02
2.091	2	041	43.23
2.075	7	$\bar{1}41, \bar{4}03$	43.58
2.060	6	123, 510	43.92
2.042	10	213, $\bar{3}23$	44.33
2.028	4	141	44.64
2.014	1	240, 232	44.97
2.000	1	$\bar{5}12$	45.30
1.971	1	402	46.00
1.956	4	430	46.39
1.942	3	$\bar{5}21$	46.74
1.929	5	$\bar{1}33, \bar{5}01$	47.07
1.924	5	$\bar{2}04, 412$	47.21
1.904	6	520, 033	47.72
1.895	4	$\bar{2}33, \bar{1}42$	47.96
1.887	4	042	48.18
1.885	3	$\bar{5}11$	48.23
1.870	2	432	48.66
1.855	3	340	49.08
1.823	3	142, 313+	50.00
1.818	1	332	50.13
1.809	3	$\bar{3}33, \bar{3}14$	50.41
1.795	5	422	50.81
1.773	<1	$\bar{6}11$	51.50
1.764	2	600, 521	51.79
1.753	2	341	52.12
1.733	2	024, $\bar{4}04$	52.79
1.718	1	150, 242	53.27
1.698	4	051	53.97
1.693	5	$\bar{4}41, 502+$	54.13
1.672	2	$\bar{6}21$	54.87
1.658	2	124	55.37
1.638	3	214	56.12
1.635	2	620	56.21

Zinc ammine bromide, $\text{Zn}(\text{NH}_3)_2\text{Br}_2$

Sample

The sample was made by dissolving Zn in hydrobromic acid and adding NH_4Br and NH_4OH .

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.650$, $N_\gamma = 1.712$

Structure

Orthorhombic, Imam (74), $Z=4$. The structure was determined by MacGillavry and Bijvoet [1936].

NBS lattice constants:

$a = 8.419(1)$

$b = 8.816(1)$

$c = 8.122(1)$

Density

(calculated) 2.856 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 2.0$

References

MacGillavry, C. H. and Bijvoet, J. M. (1936). Z. Krist. **94**, 249.

Internal standard W, $a = 3.16516 \text{ \AA}$

$\text{CuK}\alpha_1$ $\lambda = 1.54056 \text{ \AA}$; temp. 25°C

$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
6.08	30	110	14.55
5.973	35	011	14.82
4.410	55	020	20.12
4.209	13	200	21.09
4.062	95	002	21.86
3.521	25	121	25.27
3.441	19	211	25.82
3.377	19	112	26.37
3.044	50	220	29.32
2.986	100	022	29.90
2.922	13	202	30.57
2.773	3	130	32.26
2.764	4	031	32.36
2.436	20	222	36.87
2.309	11	231	38.97
2.292	6	132	39.28
2.272	5	321	39.63
2.225	7	123	40.50
2.205	7	213,040	40.89
2.105	7	400	42.93
2.062	2	141	43.87
2.030	16	004,330	44.59
1.986	1	411	45.65
1.953	10	240	46.46
1.937	2	042	46.87
1.926	3	114	47.14
1.899	3	420	47.85
1.869	5	402	48.69
1.844	6	024	49.37
1.829	2	204	49.82
1.815	4	332	50.20
1.799	6	233	50.69
1.782	3	323	51.23
1.759	19	242	51.93
1.722	10	051	53.13
1.689	8	224	54.26
1.674	1	431,143	54.78
1.596	2	251	57.72
1.5320	2	512	60.37
1.4994	3	125	61.80
1.4936	4	251,044,+	62.09
1.4774	5	053	62.85
1.4611	2	053,404	63.63
1.4356	1	334	64.90
1.4256	2	442,161	65.41
1.4075	5	244	66.36
1.3870	2	424,260	67.47
1.3821	3	062	67.74
1.3534	2	006	69.38

Zinc fluoride hydrate, $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation, at room temperature, of an aqueous solution of ZnF_2 .

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.460$, $N_\beta = 1.458$, $N_\gamma = 1.448$; 2V is medium.

Structure

Orthorhombic, $P2_1ab$ (29), $Z=4$, isostructural with $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ [Rao et al., 1965].

NBS lattice constants:

$a = 7.544(2) \text{ \AA}$

$b = 12.641(2)$

$c = 5.292(1)$

Density

(calculated) 2.309 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 2.3$

Polymorphism

Easwaran and Srinivasan [1965] found by comparison of powder patterns that $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ was isostructural with $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$. However, Penfold and Taylor [1960] reported $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ as rhombohedral. This suggests a second form of $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ exists.

References

- Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.
 Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. 13, 953.
 Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. 3, 68.

Internal standard Ag, $a = 4.08641 \text{ \AA}$ CuK α_1 $\lambda = 1.54056 \text{ \AA}$; temp. 25 °C			
$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
5.29	6	001	16.73
4.87	100	011	18.19
4.844	100	120	18.30
4.098	70	111	21.67
3.776	7	200	23.54

$d \text{ (\AA)}$	I	hkl	$2\theta (^\circ)$
3.577	5	121	24.87
3.297	6	031	27.02
3.160	25	040	28.22
3.072	4	201	29.04
3.023	9	131	29.52
2.985	40	211	29.91
2.762	20	221	32.39
2.592	10	012	34.58
2.555	12	141	35.10
2.484	3	231	36.13
2.449	6	112	36.67
2.323	10	122	38.73
2.281	4	051	39.47
2.236	14	311	40.30
2.202	3	241	40.96
2.184	14	151	41.31
2.167	16	202	41.65
2.148	3	132	42.02
2.135	4	212	42.29
2.029	16	160,042	44.62
1.999	4	331	45.32
1.957	4	061	46.35
1.952	8	251	46.49
1.927	4	232	47.13
1.887	8	400	48.19
1.845	2	341	49.36
1.804	6	312	50.54
1.786	12	242	51.09
1.759	13	411	51.94
1.751	18	322	52.20
1.738	8	261	52.63
1.709	4	071	53.59
1.689	2	351	54.25
1.673	2	332	54.84
1.667	4	171	55.06
1.658	4	123	55.36
1.644	4	252	55.88
1.619	3	440	56.83
1.615	5	360	56.97
1.610	5	162	57.18
1.589	2	133	57.96
1.581	2	080	58.32
1.579	2	342	58.41
1.557	2	271	59.29
1.544	1	361	59.85
1.541	3	043	60.02
1.537	1	402	60.19
1.4934	5	233	62.10
1.4671	5	520	63.34

Additional patterns

1. PDF card 1-253 [New Jersey Zinc Co.]

Calcium bromide, CaBr₂

Structure

Orthorhombic, Pnnm (58), Z=2. The structure was determined by Döll and Klemm [1939], and refined by Brackett et al. [1963]. It is isostructural with CaCl₂ [van Bever and Nieuwenkamp, 1935].

Lattice parameters

a=6.584(6), b=6.871(6), c=4.342(4) Å [Brackett et al., 1963].

Density

(calculated) 3.380 g/cm³

Thermal parameters

Isotropic, overall B=1.0

Scattering factors

Ca²⁺ [International Tables, 1962]

Br⁻ [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 2.474 x 10⁴

Additional patterns

1. PDF card 2-535 [Döll and Klemm, 1939]

Reference

van Bever, A.K. and Nieuwenkamp, W. (1935). Z.Krist. 90, 374.

Brackett, E.B., Brackett, T.E., and Sass, R.L. (1963) J. Inorg. Nucl. Chem. 25, 1295.

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Döll, W. and Klemm, W. (1939). Z. anorg.u.allgem. Chem. 241, 233.

International Tables for X-ray Crystallography III (1962), 204.

Calculated Pattern (Peak heights)				
<i>d</i> (Å)	<i>I</i>	<i>hkl</i>	<i>2θ</i> (°)	<i>λ</i> = 1.54056 Å
4.75	20	1 1 0	18.66	
3.672	9	0 1 1	24.22	
3.625	3	1 0 1	24.54	
3.435	1	0 2 0	25.92	
3.292	21	2 0 0	27.06	
3.206	100	1 1 1	27.80	
3.046	52	1 2 0	29.30	
2.968	1	2 1 0	30.08	
2.494	5	1 2 1	35.98	
2.451	38	2 1 1	36.64	
2.377	12	2 2 0	37.82	
2.171	15	0 0 2	41.56	
2.085	1	2 2 1	43.36	
2.026	23	0 3 1	44.70	
1.975	2	1 1 2	45.92	
1.958	3	3 0 1	46.32	
1.883	15	3 1 1	48.28	
1.850	8	3 2 0	49.22	
1.812	5	2 0 2	50.30	
1.768	15	1 2 2	51.66	
1.725	8	2 3 1	53.04	
1.662	4	1 4 0	55.22	
1.646	5	4 0 0	55.80	
1.603	5	2 2 2	57.44	
1.585	1	3 3 0	58.16	
1.552	1	1 4 1	59.50	
1.523	4	2 4 0	60.76	
1.502	1	4 1 1	61.70	
1.408	5	3 2 2	66.34	
1.404	3	4 2 1	66.52	
1.385	4	1 1 3	67.60	
1.353	1	3 4 0	69.42	
1.320	3	1 4 2	71.42	
1.312	3	4 0 2	71.92	
1.301	3	2 1 3	72.60	
1.285	4	1 5 1	73.66	
1.280	2	3 3 2	74.00	
1.278	6	4 3 1	74.16	
1.247	3	2 4 2	76.32	
1.240	2	5 1 1	76.84	
1.230	1	5 2 0	77.58	
1.223	3	0 3 3	78.04	
1.217	1	2 5 1	78.52	
1.190	2	3 1 3	80.68	
1.148	2	3 4 2	84.28	
1.147	2	2 3 3	84.38	
1.145	2	0 6 0	84.54	
1.125	2	3 5 1	86.42	
1.086	1	0 0 4	90.40	
1.070	1	5 2 2	92.10	

Calcium bromide, CaBr_2 - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.051	1	6 1 1	94.22
1.022	1	1 2 4	97.76
1.016	1	5 4 1	98.58
1.013	1	0 6 2	99.00
.985	2	1 5 3	102.84
.982	2	4 3 3	103.34
.968	1	2 6 2	105.44
.964	1	5 1 3 +	106.02
.942	1	5 4 2 +	109.76
.940	1	4 6 0	110.06
.936	1	3 2 4	110.74
.929	1	5 5 1	112.06
.919	2	2 7 1 +	113.84
.909	1	1 4 4	115.88
.907	1	3 5 3 +	116.20
.906	1	4 0 4	116.42
.884	1	2 4 4	121.24
.863	1	4 6 2	126.48
.854	1	1 1 5	128.76
.852	1	1 8 0	129.50
.851	1	6 4 2	129.74
.814	1	5 2 4	142.38
.812	1	0 3 5	143.12
.808	1	7 3 2	145.02
.802	1	3 1 5	147.68
.800	1	3 8 0	148.76
.795	1	5 5 3	151.56
.793	1	1 8 2	152.62
.789	2	2 7 3 +	155.20
.788	1	0 6 4	155.78
.787	1	8 2 1 +	156.52

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
4.75	18	1 1 0	18.65
3.671	9	0 1 1	24.23
3.625	3	1 0 1	24.54
3.435	1	0 2 0	25.91
3.292	20	2 0 0	27.06
3.206	100	1 1 1	27.80
3.046	51	1 2 0	29.30
2.969	1	2 1 0	30.08
2.493	6	1 2 1	35.99
2.451	41	2 1 1	36.64
2.377	13	2 2 0	37.82
2.171	17	0 0 2	41.56
2.085	1	2 2 1	43.36
2.026	27	0 3 1	44.70
1.975	3	1 1 2	45.92
1.959	4	3 0 1	46.32
1.936	1	1 3 1	46.89
1.884	18	3 1 1	48.28
1.850	10	3 2 0	49.23
1.812	7	2 0 2	50.30
1.768	18	1 2 2	51.66
1.725	11	2 3 1	53.03
1.718	1	0 4 0	53.29
1.662	5	1 4 0	55.22
1.646	6	4 0 0	55.81
1.603	6	2 2 2	57.44
1.585	2	3 3 0	58.17
1.552	1	1 4 1	59.50
1.523	5	2 4 0	60.77
1.502	1	4 1 1	61.71
1.408	7	3 2 2	66.34
1.405	1	4 2 1	66.51
1.385	6	1 1 3	67.60
1.353	2	3 4 0	69.42
1.347	1	0 4 2	69.75
1.320	4	1 4 2	71.42
1.312	5	4 0 2	71.93
1.301	4	2 1 3	72.61
1.285	6	1 5 1	73.66
1.280	1	3 3 2	74.00
1.277	9	4 3 1	74.17
1.247	5	2 4 2	76.32
1.239	3	5 1 1	76.85
1.230	2	5 2 0	77.58
1.224	4	0 3 3	78.04
1.217	1	2 5 1	78.51
1.190	3	3 1 3	80.68
1.183	1	5 2 1	81.25
1.148	2	3 4 2	84.28
1.147	2	2 3 3	84.39

Calcium bromide, CaBr_2 - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.145	2	0 6 0	84.54
1.125	4	3 5 1	86.43
1.111	1	5 1 2	87.78
1.086	1	0 0 4	90.41
1.082	1	2 6 0	90.82
1.070	2	5 2 2	92.10
1.051	2	6 1 1	94.22
1.045	1	5 4 0	94.96
1.031	1	2 0 4	96.70
1.022	3	1 2 4	97.76
1.016	1	5 4 1	98.60
1.013	2	0 6 2	99.01
.987	1	2 2 4	102.54
.985	3	1 5 3	102.84
.982	4	4 3 3	103.34
.968	1	2 6 2	105.44
.965	1	6 3 1	105.94
.964	2	5 1 3	106.02
.947	1	1 7 1	108.78
.942	1	6 2 2	109.74
.942	1	5 4 2	109.77
.940	2	4 6 0	110.05
.936	2	3 2 4	110.73
.929	2	5 5 1	112.07
.925	1	6 4 0	112.81
.919	3	2 7 1	113.83
.919	1	7 0 1	113.85
.911	1	7 1 1	115.43
.909	1	1 4 4	115.89
.907	2	3 5 3	116.18
.907	1	7 2 0	116.22
.906	2	4 0 4	116.43
.884	2	2 4 4	121.25
.878	1	3 7 1	122.75
.870	1	7 3 0	124.58
.867	1	6 1 3	125.25
.863	3	4 6 2	126.49
.854	2	1 1 5	128.76
.852	1	1 8 0	129.50
.851	2	6 4 2	129.75
.847	1	5 4 3	130.77
.847	1	3 4 4	130.97
.837	2	7 2 2	133.92
.833	2	2 1 5	135.09
.828	1	4 7 1	137.10
.823	1	8 0 0	138.76
.817	1	6 3 3	141.10
.814	2	5 2 4	142.37
.812	3	0 3 5	143.11
.808	2	7 3 2	145.02

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
.806	1	1 7 3	145.64
.802	3	3 1 5	147.68
.800	2	3 8 0	148.76
.798	1	6 5 2	149.96
.795	3	5 5 3	151.55
.793	4	1 8 2	152.60
.792	1	6 6 0	152.92
.789	5	2 7 3	155.18
.789	2	7 0 3	155.21
.788	3	2 3 5	155.41
.788	4	0 6 4	155.78
.787	2	8 2 1	156.27
.787	1	5 7 0	156.35
.784	3	7 1 3	158.90

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$

Structure

Triclinic, $\text{P}\bar{1}$ (2), $Z=2$. The structure was determined by Thewalt and Bugg [1973].

Lattice parameters

$a=6.593(2)$, $b=6.364(5)$, $c=8.557(3)\text{\AA}$, $\alpha=97.77(5)$, $\beta=93.52(4)$, $\gamma=110.56(3)^\circ$ [ibid.]

Density

(calculated) 1.838 g/cm^3

Thermal parameters

Anisotropic [ibid.]

Polymorphism

Three crystalline forms have been described. [Gmelins Handbuch, 1957]. The form characterized here apparently corresponds to the α -form [Thewalt and Bugg, 1973]

Scattering factors

Ca^{2+} , Cl^- [Cromer and Waber, 1965], corrected for dispersion using terms $\Delta f'$ and $\Delta f''$ from Cromer and Liberman [1970].

Scale factor

(integrated intensities) 0.2942×10^4

Additional patterns

1. PDF card 1-1080 [Hanawalt et al., 1938]

Reference

- Cromer, D.T. and Liberman, D. (1970). J.Chem.Phys. **53**, 1891.
Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. **18**, 104.
Gmelins Handbuch der Anorganischen Chemie. Calcium, Teil B (1957). Pg. 468.
Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938) Ind. Eng. Chem. Anal. Ed. **10**, 457.
Thewalt, U. and Bugg, C.E. (1973). Acta Cryst. **B29** 615.

Calculated Pattern (Peak heights)			
$d\text{ (\AA)}$	I	hkl	$2\theta(^\circ)$ $\lambda = 1.54056\text{ \AA}$
6.13	51	1 0 0	14.44
5.87	91	0 1 0	15.08
5.31	29	-1 1 0	16.68
5.25	27	-1 0 1 +	16.88
4.70	28	1 0 1	18.86
4.60	100	1 -1 1	19.28
4.48	3	0 1 1	19.82
4.40	2	-1 1 1	20.18
3.729	9	0 -1 2	23.84
3.633	15	1 1 0	24.48
3.567	53	-1 -1 1	24.94
3.383	4	1 -1 2	26.32
3.295	38	1 0 2	27.04
3.243	4	-2 1 0	27.48
3.222	16	-1 1 2	27.66
3.180	22	0 1 2	28.04
3.129	34	-1 2 0	28.50
3.064	33	2 0 0	29.12
3.056	24	1 -2 1	29.20
3.021	6	-1 -1 2	29.54
2.996	38	2 -1 1 +	29.80
2.938	62	0 2 0	30.40
2.930	42	0 -2 1	30.48
2.826	31	-1 2 1	31.64
2.806	23	0 0 3	31.86
2.778	4	2 0 1	32.20
2.715	71	0 -1 3	32.96
2.667	9	1 -2 2	33.58
2.657	22	-2 2 0	33.70
2.629	74	-2 0 2 +	34.08
2.609	21	-2 1 2	34.34
2.572	19	2 -2 1	34.86
2.535	9	1 -1 3	35.38
2.498	14	-2 2 1	35.92
2.445	6	1 0 3	36.72
2.433	10	-1 1 3 +	36.92
2.398	29	-2 -1 1	37.48
2.382	65	0 1 3 +	37.74
2.350	18	2 0 2	38.26
2.300	17	2 -2 2	39.14
2.239	22	0 2 2	40.24
2.234	20	-2 -1 2	40.34
2.224	16	1 -2 3 +	40.52
2.219	30	-1 -2 2	40.62
2.205	62	2 1 1 +	40.90
2.198	60	-2 2 2	41.02
2.193	25	-3 1 0	41.12
2.156	30	-2 1 3 +	41.86
2.105	8	0 0 4 +	42.94
2.100	8	-1 3 0	43.04

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.096	8	0 -1 4	43.12
2.090	26	2 -1 3	43.26
2.066	16	-1 0 4 +	43.78
2.055	6	1 1 3	44.02
2.041	6	-3 0 1	44.34
2.004	30	2 -3 1 +	45.20
1.999	18	-3 1 2	45.34
1.994	6	1 -3 2	45.46
1.980	6	2 -2 3 +	45.80
1.974	13	-1 3 1 +	45.94
1.958	6	0 3 0 +	46.32
1.934	1	3 0 1	46.94
1.919	7	-2 3 1	47.32
1.901	6	0 -3 2	47.80
1.897	4	3 -1 2	47.92
1.883	2	0 1 4	48.28
1.878	3	0 2 3	48.42
1.865	1	0 -2 4	48.78
1.851	3	1 -2 4	49.18
1.843	3	-2 -2 1	49.42
1.838	2	-2 0 4	49.54
1.817	5	2 2 0	50.18
1.784	5	-2 -2 2 +	51.16
1.759	6	3 0 2	51.94
1.754	7	-2 3 2 +	52.10
1.750	16	0 -3 3	52.24
1.745	9	3 1 0	52.40
1.720	1	-1 -3 1	53.20
1.716	4	2 2 1	53.36
1.696	5	0 -1 5 +	54.04
1.691	8	2 -2 4 +	54.18
1.679	4	-1 -3 2	54.60
1.675	3	-1 0 5	54.76
1.672	2	0 3 2	54.88
1.664	5	-3 2 3 +	55.14
1.659	7	3 1 1	55.34
1.647	3	2 0 4	55.76
1.635	7	-4 1 0	56.20
1.631	4	-4 1 1	56.38
1.622	9	-4 2 0	56.70
1.608	6	1 3 1	57.26
1.603	4	-4 2 1	57.44
1.592	2	-3 -1 3 +	57.88
1.582	3	4 -1 1 +	58.26
1.578	5	1 0 5 +	58.42
1.572	4	2 2 2	58.70
1.567	3	3 0 3	58.88
1.564	3	-2 4 0	59.00
1.563	3	-1 4 0	59.06
1.560	3	-3 0 4	59.16

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.555	2	-2 0 5	59.38
1.551	2	0 1 5	59.54
1.541	3	1 -4 2	59.96
1.533	3	3 -3 3 +	60.34
1.514	1	-2 1 5	61.16
1.506	1	-2 4 1	61.52
1.498	5	-4 0 2	61.90
1.493	10	-2 -1 5 +	62.14
1.484	3	1 3 2 +	62.54
1.481	3	4 -3 1	62.70
1.474	3	3 -2 4 +	63.02
1.468	8	0 4 0	63.28
1.465	6	-3 3 3 +	63.44
1.454	1	-3 -1 4	63.98
1.452	1	-1 -3 4	64.06
1.446	2	-3 -2 2	64.40
1.442	3	1 2 4	64.58
1.436	1	1 1 5	64.88
1.431	2	-3 4 1 +	65.14
1.428	3	3 -4 2	65.28
1.424	3	-4 2 3	65.48
1.420	4	0 -1 6	65.70
1.417	3	-4 0 3 +	65.88
1.414	5	1 -3 5 +	66.04
1.407	4	-4 3 2 +	66.36
1.403	6	0 0 6 +	66.58
1.391	7	-2 2 5 +	67.24
1.377	2	-2 -3 3 +	68.00
1.367	4	4 -1 3 +	68.60
1.358	7	-2 -2 5 +	69.12
1.355	5	-3 4 2	69.30
1.344	3	-4 1 4 +	69.96
1.340	2	-1 1 6	70.16
1.334	1	2 -4 4	70.54
1.331	2	4 -3 3	70.74
1.327	2	0 3 4	70.96
1.323	3	1 4 0 +	71.20
1.317	1	-1 -3 5	71.56
1.314	1	-3 -1 5	71.80
1.311	1	-1 -2 6	71.98
1.305	3	-4 -1 3 +	72.36
1.302	2	-2 4 3 +	72.54
1.297	1	3 -1 5	72.88
1.286	1	-1 4 3	73.56
1.283	4	2 1 5	73.82
1.271	1	2 2 4	74.64
1.267	1	-5 3 0	74.90
1.255	1	1 -5 1	75.74
1.254	1	3 1 4	75.82

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ – continued

Calculated Pattern (Integrated)				d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$				
6.13	46	1 0 0	14.44	2.239	25	0 2 2	40.24
5.87	86	0 1 0	15.07	2.234	18	-2 -1 2	40.35
5.31	28	-1 1 0	16.67	2.225	10	1 -2 3	40.51
5.26	16	-1 0 1	16.85	2.224	2	0 -2 3	40.53
5.25	12	0 -1 1	16.88	2.219	29	-1 -2 2	40.63
4.70	28	1 0 1	18.86	2.204	64	2 1 1	40.90
4.60	100	1 -1 1	19.28	2.203	18	-2 0 3	40.94
4.48	2	0 1 1	19.81	2.198	32	-2 2 2	41.03
4.40	2	-1 1 1	20.18	2.193	5	-3 1 0	41.12
3.731	10	0 -1 2	23.83	2.156	21	-2 1 3	41.86
3.633	16	1 1 0	24.48	2.156	3	1 2 1	41.86
3.568	57	-1 -1 1	24.94	2.156	14	-3 1 1	41.87
3.383	4	1 -1 2	26.32	2.107	1	1 -3 1	42.88
3.295	42	1 0 2	27.04	2.105	9	0 0 4	42.93
3.244	4	-2 1 0	27.47	2.100	3	-1 3 0	43.05
3.223	17	-1 1 2	27.66	2.096	5	0 -1 4	43.11
3.179	25	0 1 2	28.05	2.090	32	2 -1 3	43.25
3.143	4	1 1 1	28.37	2.067	14	-1 0 4	43.76
3.129	37	-1 2 0	28.50	2.066	8	-3 2 0	43.78
3.065	38	2 0 0	29.11	2.055	7	1 1 3	44.02
3.054	7	1 -2 1	29.22	2.041	6	-3 0 1	44.33
3.021	5	-1 -1 2	29.54	2.006	4	3 -2 1	45.16
2.995	6	-2 0 1	29.80	2.004	37	2 -3 1	45.21
2.995	37	2 -1 1	29.80	1.998	3	-3 1 2	45.36
2.937	74	0 2 0	30.41	1.993	3	1 -3 2	45.47
2.930	2	0 -2 1	30.48	1.980	5	2 -2 3	45.79
2.825	35	-1 2 1	31.64	1.978	1	-1 -2 3	45.83
2.807	24	0 0 3	31.86	1.976	5	-1 -1 4	45.89
2.777	4	2 0 1	32.20	1.973	12	-1 3 1	45.95
2.716	84	0 -1 3	32.95	1.959	3	2 0 3	46.32
2.673	3	-1 0 3	33.49	1.958	5	0 3 0	46.33
2.667	6	1 -2 2	33.57	1.934	2	3 0 1	46.93
2.657	22	-2 2 0	33.70	1.919	9	-2 3 1	47.32
2.639	2	0 2 1	33.94	1.902	7	0 -3 2	47.79
2.629	81	-2 0 2	34.07	1.896	1	3 -1 2	47.93
2.624	25	0 -2 2	34.14	1.884	2	0 1 4	48.27
2.610	20	-2 1 2	34.33	1.878	3	0 2 3	48.43
2.571	22	2 -2 1	34.86	1.866	1	0 -2 4	48.78
2.535	10	1 -1 3	35.38	1.851	4	1 -2 4	49.17
2.499	17	-2 2 1	35.91	1.843	3	-2 -2 1	49.42
2.446	7	1 0 3	36.72	1.839	1	-2 0 4	49.53
2.434	1	-1 -1 3	36.89	1.816	8	2 2 0	50.18
2.432	11	-1 1 3	36.93	1.784	7	-2 -2 2	51.16
2.397	34	-2 -1 1	37.49	1.782	1	-1 3 2	51.22
2.385	2	2 1 0	37.68	1.759	7	3 0 2	51.94
2.382	73	0 1 3	37.74	1.754	5	-2 3 2	52.10
2.380	7	-1 2 2	37.78	1.753	1	-3 0 3	52.14
2.350	21	2 0 2	38.26	1.749	20	0 -3 3	52.24
2.338	1	1 2 0	38.47	1.743	2	3 1 0	52.44
2.300	20	2 -2 2	39.14	1.722	1	-1 -3 1	53.14

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.715	5	2 2 1	53.37
1.698	2	1 1 4	53.95
1.696	4	0 -1 5	54.03
1.695	2	1 3 0	54.05
1.692	8	2 -2 4	54.17
1.689	1	2 1 3	54.25
1.679	5	-1 -3 2	54.61
1.675	1	-1 0 5	54.76
1.671	1	0 3 2	54.88
1.664	5	-3 2 3	55.14
1.663	1	3 -2 3	55.17
1.663	3	3 -3 2	55.19
1.659	8	3 1 1	55.35
1.647	3	2 0 4	55.76
1.635	10	-4 1 0	56.20
1.629	1	-4 1 1	56.43
1.622	14	-4 2 0	56.71
1.607	8	1 3 1	57.26
1.602	1	-4 2 1	57.48
1.592	3	-3 -1 3	57.88
1.589	1	0 2 4	57.98
1.583	1	-1 1 5	58.25
1.582	2	4 -1 1	58.27
1.580	2	0 -2 5	58.37
1.579	2	1 -4 1	58.39
1.577	2	1 0 5	58.47
1.572	4	2 2 2	58.70
1.567	1	3 0 3	58.90
1.564	3	-2 4 0	58.99
1.563	1	-1 4 0	59.07
1.561	2	-3 0 4	59.15
1.555	2	-2 0 5	59.39
1.551	1	0 1 5	59.54
1.542	4	1 -4 2	59.96
1.533	2	3 -3 3	60.32
1.533	2	4 0 0	60.34
1.514	1	-2 1 5	61.15
1.506	1	-2 4 1	61.51
1.498	4	-4 0 2	61.90
1.498	2	4 -2 2	61.90
1.493	7	0 3 3	62.13
1.492	8	-2 -1 5	62.15
1.485	1	4 -1 2	62.47
1.484	4	1 3 2	62.55
1.480	2	4 -3 1	62.70
1.478	1	4 0 1	62.84
1.476	1	2 -1 5	62.93
1.474	2	3 -2 4	63.01
1.473	1	3 -1 4	63.07
1.469	12	0 4 0	63.27

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.465	2	-3 3 3	63.42
1.464	1	-4 1 3	63.50
1.454	1	-3 -1 4	63.98
1.452	1	-1 -3 4	64.06
1.446	2	-3 -2 2	64.40
1.442	4	1 2 4	64.59
1.436	1	1 1 5	64.89
1.431	1	2 3 0	65.14
1.431	2	-3 4 1	65.14
1.428	4	3 -4 2	65.28
1.424	3	-4 2 3	65.50
1.420	5	0 -1 6	65.71
1.417	1	2 2 3	65.86
1.417	1	-4 0 3	65.86
1.414	5	1 -3 5	66.04
1.413	3	-2 4 2	66.09
1.408	2	2 0 5	66.34
1.407	4	-4 3 2	66.38
1.403	7	0 0 6	66.58
1.401	1	0 -4 3	66.69
1.392	4	-1 3 4	67.17
1.391	9	-2 2 5	67.23
1.379	1	-3 1 5	67.94
1.377	3	-2 -3 3	68.00
1.367	6	4 -1 3	68.59
1.365	1	0 2 5	68.69
1.358	4	-4 -1 2	69.09
1.358	1	0 -2 6	69.12
1.358	5	-2 -2 5	69.13
1.358	3	2 -3 5	69.13
1.355	2	-3 4 2	69.26
1.344	1	-1 -4 1	69.93
1.343	4	-4 1 4	69.97
1.340	2	-1 1 6	70.15
1.334	1	2 -4 4	70.55
1.331	2	4 -3 3	70.74
1.327	2	0 3 4	70.97
1.323	2	1 4 0	71.19
1.323	1	-3 3 4	71.20
1.317	1	-1 -3 5	71.56
1.314	1	-3 -1 5	71.80
1.311	1	-1 -2 6	71.98
1.305	2	-4 2 4	72.36
1.305	2	-4 -1 3	72.37
1.303	1	-2 1 6	72.48
1.302	1	-2 4 3	72.53
1.300	1	-5 1 1	72.65
1.297	1	3 -1 5	72.89
1.286	1	-1 4 3	73.56
1.283	5	2 1 5	73.82

Chromium chloride, CrCl₂

Structure

Orthorhombic, Pnmm (58), Z=2 [Handy and Gregory, [1951]. The structure was determined independently and practically at the same time in four different laboratories and reported jointly in one paper [Tracy et al., 1961]

Lattice parameters

a=6.631, b=5.980, c=3.487Å [Tracy et al., 1961]

Density

(calculated) 2.952 g/cm³

Thermal parameters

Anisotropic; $\beta_{11}=0.0137$, $\beta_{22}=0.0119$ for all atoms

Atomic positions

Cr in 2a: 0,0,0

Cl in 4g: x,y,0 with x=0.360, y=0.275

Scattering factors

Cr²⁺, Cl⁻ [Berghuis et al., 1955]

Scale factor

(integrated intensities) 0.5267 x 10⁴

Additional patterns

1. PDF card 6-0159 [Handy and Gregory, 1951].

2. Oswald [1961]

Reference

Berghuis, J., Haanapel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H., and Veenendahl, A. L. (1955). Acta Cryst. 8, 478.

Handy, L. L. and Gregory, N. W. (1951). J. Chem. Phys. 19, 1314.

Oswald, H. R. (1961). Helv. Chim. Acta 44, 1049.

Tracy, J.W., Gregory, N.W., Lingafelter, E.C., Dunitz, J.D., Mez, H.-C., Rundle, R.E., Scheringer, C., Yakel, H.L., Jr., and Wilkinson, M.K. (1961). Acta Cryst. 14, 927.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ \AA}$
4.44	100	1 1 0	19.98
3.314	8	2 0 0	26.88
3.011	15	0 1 1	29.64
2.990	2	0 2 0	29.86
2.899	36	2 1 0	30.82
2.743	41	1 1 1	32.62
2.230	19	2 1 1	40.42
2.220	15	2 2 0	40.60
2.147	49	1 2 1	42.04
2.073	4	3 1 0	43.62
1.909	2	1 3 0	47.60
1.873	2	2 2 1	48.58
1.867	18	3 0 1	48.74
1.782	2	3 1 1	51.22
1.743	10	0 0 2	52.44
1.731	8	0 3 1	52.86
1.708	3	2 3 0	53.60
1.674	4	1 3 1	54.78
1.623	6	1 1 2	56.68
1.543	1	2 0 2	59.88
1.534	3	2 3 1	60.28
1.494	8	2 1 2 +	62.06
1.480	3	3 3 0	62.72
1.452	4	4 1 1	64.06
1.450	6	4 2 0	64.18
1.371	3	2 2 2	68.36
1.363	1	3 3 1 +	68.84
1.334	1	3 1 2	70.52
1.269	1	2 4 1	74.72
1.240	1	5 0 1	76.84
1.220	2	2 3 2	78.28
1.214	1	5 1 1	78.78
1.177	1	1 5 0	81.76
1.167	3	3 4 1	82.62
1.135	2	0 4 2	85.48
1.128	2	3 3 2	86.10
1.125	2	1 1 3	86.46
1.115	3	4 2 2	87.42
1.079	1	2 1 3	91.12
1.071	1	2 5 1	92.02
1.069	3	1 2 3	92.18
1.029	2	3 0 3	96.96
1.004	1	0 3 3	100.20
.976	1	1 5 2	104.30
.934	1	4 5 1	111.04
.933	1	6 0 2	111.24
.933	1	5 3 2	111.32
.874	1	7 2 1 +	123.56
.872	1	0 0 4	124.14
.855	1	1 1 4	128.44
.848	1	3 4 3	130.70
.845	1	6 3 2	131.34

Chromium chloride, CrCl_2 - continued

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
4.44	100	1 1 0	19.98
3.315	9	2 0 0	26.87
3.012	18	0 1 1	29.63
2.990	1	0 2 0	29.86
2.900	43	2 1 0	30.81
2.743	48	1 1 1	32.62
2.726	2	1 2 0	32.83
2.230	23	2 1 1	40.42
2.220	15	2 2 0	40.60
2.147	62	1 2 1	42.04
2.073	5	3 1 0	43.62
1.909	2	1 3 0	47.60
1.873	2	2 2 1	48.57
1.867	24	3 0 1	48.74
1.782	3	3 1 1	51.22
1.743	14	0 0 2	52.44
1.731	11	0 3 1	52.86
1.708	5	2 3 0	53.60
1.674	6	1 3 1	54.78
1.623	10	1 1 2	56.67
1.543	2	2 0 2	59.89
1.534	4	2 3 1	60.28
1.495	4	0 4 0	62.03
1.494	9	2 1 2	62.06
1.480	4	3 3 0	62.71
1.452	5	4 1 1	64.06
1.450	7	4 2 0	64.19
1.371	5	2 2 2	68.35
1.363	1	2 4 0	68.83
1.363	1	3 3 1	68.85
1.334	2	3 1 2	70.52
1.295	1	5 1 0	73.02
1.287	1	1 3 2	73.50
1.269	1	2 4 1	74.72
1.240	2	5 0 1	76.84
1.220	3	2 3 2	78.29
1.214	2	5 1 1	78.78
1.177	2	1 5 0	81.75
1.167	5	3 4 1	82.61
1.135	3	0 4 2	85.49
1.128	3	3 3 2	86.10
1.124	2	1 1 3	86.48
1.115	6	4 2 2	87.42
1.079	2	2 1 3	91.12
1.074	1	2 4 2	91.68
1.071	1	2 5 1	92.01
1.069	6	1 2 3	92.18
1.053	1	5 3 1	94.07
1.039	1	5 1 2	95.64
1.029	3	3 0 3	96.96

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.004	2	0 3 3	100.20
.993	1	1 3 3	101.77
.976	2	1 5 2	104.30
.961	1	2 3 3	106.56
.954	1	5 4 1	107.65
.948	2	1 6 1	108.61
.945	1	2 5 2	109.14
.940	1	4 1 3	110.08
.934	2	4 5 1	111.04
.933	1	6 0 2	111.22
.933	1	5 3 2	111.33
.931	1	6 3 1	111.58
.922	1	6 1 2	113.27
.921	1	2 6 1	113.59
.884	1	2 4 3	121.15
.874	2	7 2 1	123.55
.874	1	5 0 3	123.58
.872	3	0 0 4	124.16
.865	2	5 1 3	125.89
.855	2	1 1 4	128.44
.854	1	4 6 0	128.79
.847	4	3 4 3	130.71
.845	1	6 3 2	131.35
.837	1	2 6 2	133.86
.835	4	2 1 4	134.64
.830	2	0 7 1	136.35
.827	1	1 5 3	137.30
.824	1	7 1 2	138.24
.811	3	2 2 4	143.34
.808	2	2 5 3	144.68
.804	1	3 1 4	146.89
.801	2	5 3 3	148.40
.797	2	3 7 0	150.33
.794	1	6 1 3	152.02
.793	1	1 3 4	152.52
.792	2	6 4 2	153.24

Copper aluminum, Cu₉Al₄

Structure

Cubic, $P\bar{4}3m$ (215), $Z=4$. The structure was determined by Bradley and Jones [1933]. It was refined first by Westman [1965] and later by Heidenstam, Johansson, and Westman [1968]. This is the same phase of the copper-aluminum system that was called δ -CuAl (or Cu₉Al₄) by Bradley and Jones [1933] and by Weibke [1934]; it was later called γ -Cu₉Al₄ by Westman [1965] because its structure is very similar to that of γ -brass.

Lattice parameters

$a=8.7027(5)\text{\AA}$ (published value: $8.7023(5)\text{\AA}$) [Heidenstam et al., 1968]

Density

(calculated) 6.850 g/cm^3

Thermal parameters

Isotropic [Heidenstam et al., 1968]

Atomic positions

The parameter values used were those in table 5 [Heidenstam et al., 1968], with half the "octahedral" Cu atoms in positions 6f and the other half in positions 6g [Westman, 1965].

Scattering factors

Cu⁰, Al⁰ [Cromer and Waber, 1965]: all factors were corrected for dispersion [Cromer, 1965].

Scale factor

(integrated intensities) 63.01×10^4

Additional patterns

1. PDF card 2-1254 [Weibke, 1934]

References

- Bradley, A.J., and Jones, P. (1934). J. Inst. Metals 51, 131.
Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
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v. Heidenstam, O., Johansson, A., and Westman, S. (1968). Acta Chem. Scand. 22, 653.
Weibke, F. (1934). Z. anorg.u.allgem. Chem. 220, 293.
Westman, S. (1965). Acta Chem. Scand. 19, 1411.

Calculated Pattern (Peak heights)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ \AA}$
8.699	3	1 0 0	10.16
6.154	1	1 1 0	14.38
3.8903	4	2 1 0	22.84
3.5533	8	2 1 1	25.04
2.9006	8	3 0 0 +	30.80
2.5116	2	2 2 2	35.72
2.3259	3	3 2 1	38.68
2.0509	100	3 3 0 +	44.12
1.8990	1	4 2 1	47.86
1.8553	4	3 3 2	49.06
1.7762	4	4 2 2	51.40
1.7066	1	5 1 0 +	53.66
1.6749	1	5 1 1 +	54.76
1.5150	1	5 2 2	61.12
1.4503	8	6 0 0 +	64.16
1.4116	2	6 1 1 +	66.14
1.2832	2	6 3 1	73.78
1.2562	3	4 4 4	75.64
1.2306	2	5 5 0 +	77.50
1.1844	12	6 3 3 +	81.14
1.1053	1	7 3 2	88.36
1.0712	5	7 4 1	91.96
1.0553	1	8 2 0 +	93.76
1.0256	2	6 6 0 +	97.36
.9173	2	9 3 0 +	114.22
.8791	3	8 5 3 +	122.38
.8617	1	10 1 1 +	126.74
.8374	1	10 2 2 +	133.80
.8151	4	7 7 4 +	141.82
.7944	2	10 4 2	151.66

Copper aluminum, Cu₉Al₄ - continued

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
8.703	3	1 0 0	10.16
6.154	1	1 1 0	14.38
3.8920	5	2 1 0	22.83
3.5529	10	2 1 1	25.04
2.9009	6	3 0 0	30.80
2.9009	4	2 2 1	30.80
2.5123	4	2 2 2	35.71
2.3259	4	3 2 1	38.68
2.1107	1	3 2 2	42.81
2.0513	100	3 3 0	44.11
2.0513	53	4 1 1	44.11
1.9460	1	4 2 0	46.64
1.8991	1	4 2 1	47.86
1.8554	6	3 3 2	49.06
1.7764	6	4 2 2	51.39
1.7067	1	4 3 1	53.66
1.7067	1	5 1 0	53.66
1.6748	1	5 1 1	54.76
1.6748	1	3 3 3	54.76
1.6161	1	4 3 2	56.93
1.5150	1	5 2 2	61.12
1.4505	8	6 0 0	64.15
1.4505	6	4 4 2	64.15
1.4118	2	6 1 1	66.13
1.4118	1	5 3 2	66.13
1.2831	3	6 3 1	73.78
1.2561	6	4 4 4	75.65
1.2307	3	5 5 0	77.49
1.2307	1	5 4 3	77.49
1.2069	1	6 4 0	79.32
1.1843	11	7 2 1	81.15
1.1843	1	5 5 2	81.15
1.1843	14	6 3 3	81.15
1.1629	1	6 4 2	82.96
1.1052	2	7 3 2	88.36
1.0712	12	7 4 1	91.95
1.0554	1	8 2 0	93.75
1.0554	1	6 4 4	93.75
1.0256	1	8 2 2	97.36
1.0256	4	6 6 0	97.36
.9983	2	6 6 2	101.00
.9854	2	7 5 2	102.83
.9174	3	9 3 0	114.21
.9174	2	7 5 4	114.21
.8791	2	9 4 1	122.38
.8791	6	8 5 3	122.38
.8617	1	7 7 2	126.74
.8617	3	10 1 1	126.74
.8534	2	8 6 2	129.01
.8453	1	9 4 3	131.36

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
.8374	3	10 2 2	133.80
.8374	1	6 6 6	133.80
.8298	1	9 5 2	136.34
.8151	2	8 7 1	141.83
.8151	12	7 7 4	141.83
.8151	2	8 5 5	141.83
.8046	1	8 7 2	146.43
.8046	1	10 4 1	146.43
.8012	1	10 3 3	148.09
.8012	2	9 6 1	148.09
.7944	10	10 4 2	151.66
.7879	2	9 5 4	155.72
.7879	2	11 1 0	155.72

Copper cadmium, Cu₅Cd₈

Structure

Cubic, $I\bar{4}3m$ (217), $Z=4$. The structure was determined by Bradley and Gregory [1931] and refined by Heidenstam et al., [1968].

Lattice parameters

$a=9.5892(3)\text{\AA}$ (published value: $9.5888(3)\text{\AA}$) [Heidenstam et al., 1968]

Density

(calculated) 9.166 g/cm^3

Thermal parameters

Isotropic [Heidenstam et al., 1968]

Atomic positions

Cu(1) in 8c, Cu(2) in 8c. The 12(Cu,Cd) in 12e and 24(Cu,Cd) in 24g are in random arrangement in each site, in the ratio of 1 Cu to 8 Cd.

Scattering factors

Cu^0 , Cd^0 [Cromer and Waber, 1965]. All factors were corrected for dispersion [Cromer, 1965].

Scale factor

(integrated intensities) 159.5×10^4

Reference

- Bradley, A.J. and Gregory, C.H. (1931). Phil. Mag. 12, 143.
Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
Cromer, D.T. (1965). Acta Cryst. 18, 17.
v. Heidenstam, O., Johansson, A., and Westman, S. (1968). Acta Chem. Scand. 22, 653.

Calculated Pattern (<i>Peak heights</i>)			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
3.9140	1	2 1 1	22.70
3.0315	9	3 1 0	29.44
2.7676	9	2 2 2	32.32
2.5630	14	3 2 1	34.98
2.3976	1	4 0 0	37.48
2.2597	100	4 1 1 +	39.86
2.0448	12	3 3 2	44.26
1.9577	7	4 2 2	46.34
1.8805	3	5 1 0 +	48.36
1.6445	1	5 3 0 +	55.86
1.5984	3	4 4 2 +	57.62
1.5556	2	5 3 2 +	59.36
1.5163	1	6 2 0	61.06
1.4797	2	5 4 1	62.74
1.4455	1	6 2 2	64.40
1.4139	4	6 3 1	66.02
1.3839	4	4 4 4	67.64
1.3562	4	5 5 0 +	69.22
1.3048	10	7 2 1 +	72.36
1.2814	1	6 4 2	73.90
1.2177	2	7 3 2 +	78.48
1.1803	2	7 4 1	81.48
1.1629	1	8 2 0 +	82.96
1.1301	1	6 6 0 +	85.94
1.1000	1	6 6 2	88.90
1.0857	2	7 5 2	90.38
1.0107	1	8 5 1 +	99.30
.9687	2	8 5 3 +	105.34
.9228	1	10 2 2 +	113.18
.8981	1	7 7 4 +	118.12
.8543	3	10 5 1 +	128.76
.8284	1	11 3 2 +	136.82

Copper cadmium, Cu₅Cd₈ - continued

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
3.9148	1	2 1 1	22.70
3.0324	15	3 1 0	29.43
2.7682	15	2 2 2	32.31
2.5628	24	3 2 1	34.98
2.3973	2	4 0 0	37.48
2.2602	88	3 3 0	39.85
2.2602	100	4 1 1	39.85
2.0444	23	3 3 2	44.27
1.9574	14	4 2 2	46.35
1.8806	4	5 1 0	48.36
1.8806	2	4 3 1	48.36
1.7507	1	5 2 1	52.20
1.6445	2	5 3 0	55.86
1.6445	1	4 3 3	55.86
1.5982	2	6 0 0	57.63
1.5982	5	4 4 2	57.63
1.5556	1	6 1 1	59.36
1.5556	3	5 3 2	59.36
1.5162	2	6 2 0	61.07
1.4797	5	5 4 1	62.74
1.4456	3	6 2 2	64.39
1.4138	9	6 3 1	66.02
1.3841	9	4 4 4	67.63
1.3561	1	5 4 3	69.22
1.3561	7	5 5 0	69.22
1.3049	18	7 2 1	72.35
1.3049	1	5 5 2	72.35
1.3049	7	6 3 3	72.35
1.2814	2	6 4 2	73.90
1.2178	3	6 5 1	78.47
1.2178	3	7 3 2	78.47
1.1987	1	8 0 0	79.98
1.1804	5	7 4 1	81.47
1.1629	2	8 2 0	82.97
1.1629	2	6 4 4	82.97
1.1461	2	6 5 3	84.45
1.1301	2	6 6 0	85.94
1.1301	2	8 2 2	85.94
1.1000	3	6 6 2	88.90
1.0858	5	7 5 2	90.38
1.0590	1	8 3 3	93.34
1.0340	1	9 2 1	96.31
1.0108	1	7 5 4	99.29
1.0108	1	8 5 1	99.29
.9891	1	9 3 2	102.30
.9787	1	8 4 4	103.82
.9687	2	9 4 1	105.35
.9687	5	8 5 3	105.35
.9495	1	10 1 1	108.44
.9314	2	9 5 0	111.59

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
.9227	4	10 2 2	113.19
.9227	1	6 6 6	113.19
.8981	2	8 7 1	118.11
.8981	3	7 7 4	118.11
.8981	1	8 5 5	118.11
.8682	2	9 5 4	125.06
.8543	2	11 2 1	128.76
.8543	5	9 6 3	128.76
.8543	6	10 5 1	128.76
.8476	2	8 8 0	130.68
.8410	1	9 7 0	132.66
.8346	1	10 4 4	134.71
.8284	2	11 3 2	136.83
.8284	1	7 7 6	136.83
.8223	1	10 6 0	139.03
.8223	1	8 6 6	139.03
.8163	1	8 7 5	141.34
.8163	1	11 4 1	141.34
.8047	2	9 6 5	146.36
.7991	2	8 8 4	149.13
.7936	1	9 7 4	152.15
.7936	1	11 5 0	152.15
.7936	1	12 1 1	152.15
.7936	1	11 4 3	152.15
.7829	2	11 5 2	159.35

Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$

Structure

Orthorhombic, $\text{P2}_1\text{2}_1\text{2}_1$ (19), $Z=4$. The structure was determined by Handlovic [1969].

Lattice parameters

$a=6.71$, $b=9.00$, $c=7.40\text{\AA}$ [ibid.]

Density

(calculated) 2.67 g/cm^3

Thermal parameters

Isotropic [Handlovic]

Scattering factors

Cu^0 , O^0 , P^0 [International Tables, 1962]

Scale factor

(integrated intensities) 4.158×10^4

Reference

Handlovic, M. (1969). Acta Cryst. **B25**, 227
International Tables for X-ray Crystallography III
(1962). 202, 210.

Calculated Pattern (<i>Peak heights</i>)					
<i>d</i> (Å)	<i>I</i>	<i>hkl</i>			$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ \AA}$
5.38	22	1	1	0	16.46
4.97	100	1	0	1	17.84
4.50	3	0	2	0	19.72
4.35	10	1	1	1	20.40
3.84	16	0	2	1	23.12
3.74	63	1	2	0	23.80
3.70	10	0	0	2	24.04
3.422	21	0	1	2	26.02
3.336	13	1	2	1	26.70
3.241	7	1	0	2	27.50
2.893	10	2	1	1 +	30.88
2.857	2	0	2	2	31.28
2.779	7	0	3	1	32.18
2.690	9	2	2	0	33.28
2.629	8	1	2	2	34.08
2.569	4	1	3	1	34.90
2.528	38	2	2	1	35.48
2.485	2	2	0	2	36.12
2.395	5	2	1	2	37.52
2.379	1	0	1	3	37.78
2.331	1	0	3	2	38.60
2.316	9	1	0	3	38.86
2.250	4	0	4	0	40.04
2.242	5	1	1	3	40.18
2.237	4	2	3	0	40.28
2.170	3	3	1	0	41.58
2.163	7	0	2	3	41.72
2.152	3	0	4	1	41.94
2.141	4	3	0	1	42.18
2.134	5	1	4	0	42.32
2.059	4	1	2	3	43.94
2.050	7	1	4	1	44.14
2.003	6	3	2	0	45.24
1.940	2	2	1	3	46.78
1.933	2	3	2	1	46.96
1.914	3	3	0	2 +	47.46
1.905	2	0	3	3	47.70
1.869	1	2	4	0	48.68
1.848	5	1	4	2 +	49.26
1.833	4	1	3	3	49.70
1.818	3	2	2	3	50.14
1.812	5	2	4	1 +	50.32
1.793	1	3	3	0	50.88
1.783	1	1	0	4	51.18
1.762	4	3	2	2	51.86
1.750	4	1	1	4	52.24
1.745	2	3	3	1	52.40
1.711	1	0	2	4	53.52
1.693	2	1	5	1	54.14
1.678	5	4	0	0	54.66

Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.668	6	2 4 2	55.00
1.663	4	0 4 3	55.18
1.658	6	1 2 4 +	55.38
1.649	1	4 1 0	55.68
1.630	1	3 1 3	56.42
1.620	3	2 0 4	56.78
1.614	3	1 4 3	57.02
1.594	2	2 1 4	57.78
1.586	1	3 4 0	58.10
1.573	2	1 5 2 +	58.62
1.555	1	3 2 3	59.40
1.551	3	3 4 1	59.56
1.537	1	4 2 1	60.14
1.528	1	4 0 2	60.56
1.506	1	4 1 2	61.52
1.490	2	2 4 3	62.28
1.458	2	3 4 2 +	63.78
1.454	2	0 5 3	63.98
1.450	2	3 3 3	64.16
1.447	2	4 2 2	64.34
1.436	3	1 6 1 +	64.88
1.425	3	2 3 4 +	65.42
1.408	1	3 1 4	66.34
1.398	1	1 4 4	66.88
1.390	2	0 6 2	67.30
1.369	2	2 6 0	68.46
1.361	1	4 3 2 +	68.92
1.359	2	3 2 4	69.06
1.345	1	4 4 0	69.88
1.339	1	2 1 5	70.24
1.334	1	2 5 3 +	70.52
1.325	2	4 2 3	71.06
1.322	1	4 4 1	71.26
1.320	2	5 0 1	71.38
1.315	1	2 4 4	71.74
1.306	1	5 1 1	72.26
1.302	1	1 3 5	72.54
1.297	2	2 2 5	72.88
1.286	1	5 2 0	73.60
1.284	2	2 6 2	73.70
1.281	1	0 6 3	73.90
1.267	2	5 2 1 +	74.88
1.259	2	1 6 3 +	75.44
1.228	1	3 6 1	77.66
1.216	1	1 4 5	78.62
1.141	1	3 3 5 +	84.88
1.112	1	0 8 1 +	87.68
1.074	1	6 2 1	91.68
1.070	1	4 6 2	92.04
1.063	1	1 8 2	92.90
1.006	1	1 5 6	99.96

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
5.38	21	1 1 0	16.46
4.97	100	1 0 1	17.83
4.50	3	0 2 0	19.71
4.35	10	1 1 1	20.39
3.84	17	0 2 1	23.11
3.74	70	1 2 0	23.79
3.70	9	0 0 2	24.03
3.422	23	0 1 2	26.02
3.355	1	2 0 0	26.55
3.336	14	1 2 1	26.70
3.240	8	1 0 2	27.51
3.056	3	2 0 1	29.20
3.049	10	1 1 2	29.27
2.893	11	2 1 1	30.88
2.858	2	0 2 2	31.27
2.780	9	0 3 1	32.17
2.690	11	2 2 0	33.28
2.629	10	1 2 2	34.07
2.568	4	1 3 1	34.90
2.528	45	2 2 1	35.48
2.485	3	2 0 2	36.11
2.396	6	2 1 2	37.51
2.379	1	0 1 3	37.78
2.330	1	0 3 2	38.60
2.315	11	1 0 3	38.87
2.250	5	0 4 0	40.04
2.242	5	1 1 3	40.19
2.236	2	2 3 0	40.30
2.171	3	3 1 0	41.57
2.163	8	0 2 3	41.72
2.153	3	0 4 1	41.93
2.141	5	3 0 1	42.17
2.133	5	1 4 0	42.33
2.059	5	1 2 3	43.94
2.050	9	1 4 1	44.15
2.003	8	3 2 0	45.24
1.941	3	2 1 3	46.77
1.933	2	3 2 1	46.96
1.914	2	3 0 2	47.46
1.914	1	2 3 2	47.46
1.905	2	0 3 3	47.69
1.869	2	2 4 0	48.69
1.850	3	0 0 4	49.21
1.848	5	1 4 2	49.27
1.833	5	1 3 3	49.70
1.818	3	2 2 3	50.14
1.812	1	0 1 4	50.31
1.812	5	2 4 1	50.32
1.793	1	3 3 0	50.88
1.783	1	1 0 4	51.18

Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.761	6	3 2 2	51.87
1.749	5	1 1 4	52.25
1.743	1	3 3 1	52.46
1.711	2	0 2 4	53.51
1.692	2	1 5 1	54.15
1.677	8	4 0 0	54.67
1.668	8	2 4 2	55.01
1.662	1	0 4 3	55.21
1.658	6	1 2 4	55.37
1.657	2	3 0 3	55.41
1.649	1	4 1 0	55.69
1.630	2	3 1 3	56.42
1.620	4	2 0 4	56.78
1.614	3	1 4 3	57.03
1.594	2	2 1 4	57.78
1.586	2	3 4 0	58.10
1.575	1	0 3 4	58.57
1.573	3	1 5 2	58.62
1.555	1	3 2 3	59.39
1.551	4	3 4 1	59.55
1.538	2	4 2 1	60.13
1.528	1	4 0 2	60.55
1.506	2	4 1 2	61.51
1.490	4	2 4 3	62.28
1.458	2	3 4 2	63.79
1.458	1	2 5 2	63.79
1.454	1	0 5 3	63.98
1.450	2	3 3 3	64.16
1.447	1	4 2 2	64.34
1.436	1	4 3 1	64.86
1.436	4	1 6 1	64.88
1.427	1	1 1 5	65.34
1.425	3	2 3 4	65.42
1.408	2	3 1 4	66.33
1.398	2	1 4 4	66.89
1.390	2	0 6 2	67.30
1.369	3	2 6 0	68.46
1.361	1	4 3 2	68.91
1.361	1	1 6 2	68.93
1.359	3	3 2 4	69.06
1.345	1	4 4 0	69.89
1.339	2	2 1 5	70.23
1.334	1	3 4 3	70.53
1.334	1	2 5 3	70.53
1.326	3	4 2 3	71.05
1.323	1	4 4 1	71.20
1.320	2	5 0 1	71.37
1.315	2	2 4 4	71.73
1.306	1	5 1 1	72.26
1.302	2	1 3 5	72.54

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.297	4	2 2 5	72.89
1.286	1	5 2 0	73.59
1.284	2	2 6 2	73.71
1.282	1	0 6 3	73.89
1.267	1	5 2 1	74.88
1.267	1	1 5 4	74.89
1.259	1	4 3 3	75.44
1.259	1	1 6 3	75.45
1.249	1	5 1 2	76.13
1.228	2	5 6 1	77.66
1.216	1	1 4 5	78.61
1.204	1	3 4 4	79.53
1.179	1	5 0 3	81.60
1.169	1	5 1 3	82.45
1.143	1	0 5 5	84.72
1.142	1	2 7 2	84.83
1.141	1	3 3 5	84.88
1.141	1	0 3 6	84.95
1.124	1	1 7 3	86.52
1.112	2	0 8 1	87.67
1.112	1	3 6 3	87.69
1.074	1	6 2 1	91.67
1.072	1	3 1 6	91.83
1.070	1	4 6 2	92.05
1.063	2	1 8 2	92.90
1.018	1	4 6 3	98.29
1.006	1	1 5 6	99.95
1.002	2	2 1 7	100.48
.991	1	5 6 1	102.00
.986	1	1 3 7	102.71
.979	1	2 8 3	103.77
.970	1	3 8 2	105.16
.967	1	6 4 2	105.66
.945	1	4 5 5	109.25
.944	1	5 3 5	109.42

L-Cysteine, $\text{HSCH}_2\text{-CH(NH}_2\text{)COOH}$

Structure

Monoclinic, $P2_1(4)$, $Z=4$. The structure was determined by Harding and Long [1968].

Lattice parameters

$a=11.51(1)$, $b=5.240(5)$, $c=9.517(10)\text{\AA}$, $\beta=109.13^\circ$ [ibid.]

Density

(calculated) 1.484 g/cm^3

Thermal parameters

Isotropic:	carbon (1)	1.26
	" (11)	1.26
sulfur (1) $B=3.81$	nitrogen (1)	1.26
sulfur (2)	" (11)	1.74
carbon (3)	oxygen (1)	1.58
" (13)	" (11)	1.74
" (2)	" (2)	2.45
" (12)	" (12)	2.45
	hydrogen (all)	1.42

Scattering factors

C^0 , H^0 , N^0 , $\text{O}^{-1/2}$, S^0 . The sulfur factors were corrected for the real part of the dispersion. [International Tables, 1962].

Scale factor

(integrated intensities) 0.5947×10^4

Additional patterns

1. PDF card 13-722 [Eli Lilly Co., Indianapolis, Indiana.]

Reference

Harding, M.M. and Long, H.A. (1968). Acta Cryst. B24, 1096.

International Tables for X-ray Crystallography III (1962), 202, 214.

Calculated Pattern (Peak heights)			
$d\text{ (\AA)}$	I	hkl	$2\theta(^\circ)$ $\lambda = 1.54056\text{ \AA}$
10.88	42	1 0 0	8.12
8.98	4	0 0 1	9.84
8.40	1	-1 0 1	10.52
6.02	3	1 0 1	14.70
5.52	2	-2 0 1	16.04
5.43	11	2 0 0	16.30
4.72	86	1 1 0 +	18.78
4.53	100	0 1 1	19.60
4.49	92	0 0 2	19.74
4.45	34	-1 1 1	19.94
4.21	14	-2 0 2	21.10
3.96	14	1 1 1	22.46
3.82	4	-3 0 1	23.24
3.802	15	-2 1 1	23.38
3.773	29	2 1 0	23.56
3.745	41	1 0 2	23.74
3.625	44	3 0 0	24.54
3.515	54	-1 1 2	25.32
3.422	34	-3 0 2	26.02
3.411	51	0 1 2	26.10
3.281	20	-2 1 2	27.16
3.227	58	2 1 1	27.62
3.166	4	-1 0 3	28.16
3.087	15	-2 0 3 +	28.90
3.046	3	1 1 2	29.30
3.035	3	3 0 1	29.40
2.996	7	0 0 3	29.60
2.980	53	3 1 0	29.96
2.866	4	-3 1 2	31.18
2.805	1	-3 0 3	31.88
2.761	19	-4 0 2	32.40
2.719	50	4 0 0	32.92
2.712	41	-1 1 3	33.00
2.673	3	1 0 3	33.50
2.660	25	-2 1 3	33.66
2.626	7	3 1 1	34.12
2.620	11	0 2 0	34.20
2.612	11	2 1 2	34.30
2.605	6	0 1 3	34.40
2.547	9	1 2 0	35.20
2.516	4	0 2 1	35.66
2.502	3	-1 2 1	35.86
2.473	7	-3 1 3	36.30
2.456	14	3 0 2	36.56
2.443	8	-4 1 2	36.76
2.412	2	4 1 0	37.24
2.403	2	1 2 1	37.40
2.394	2	4 0 1	37.54
2.382	17	1 1 3	37.74
2.370	9	-2 0 4	37.94

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.360	6	2 2 0 +	38.10
2.293	2	-1 2 2 +	39.26
2.273	6	-3 0 4	39.62
2.248	11	0 0 4	40.08
2.221	15	-4 1 3 +	40.58
2.208	2	2 2 1	40.84
2.177	4	4 1 1	41.44
2.161	5	-3 2 1 +	41.76
2.155	3	-1 1 4	41.88
2.146	4	1 2 2	42.06
2.121	5	-5 0 3 +	42.58
2.104	2	-4 0 4	42.96
2.100	2	-5 1 1	43.04
2.085	6	-3 1 4 +	43.36
2.081	8	-3 2 2	43.46
2.066	1	0 1 4	43.78
2.048	1	4 0 2	44.18
2.019	1	-1 2 3	44.86
2.009	1	3 0 3	45.10
1.998	1	-2 2 3	45.36
1.983	4	3 2 1	45.72
1.977	13	2 2 2	45.86
1.972	9	5 0 1 +	45.98
1.967	3	-5 1 3	46.12
1.952	1	-4 1 4	46.48
1.937	1	-4 2 1	46.86
1.926	1	1 1 4	47.16
1.915	2	-3 2 3	47.44
1.907	7	4 1 2	47.64
1.901	7	-4 2 2	47.82
1.886	1	4 2 0	48.20
1.875	2	3 1 3 +	48.50
1.871	3	1 2 3 +	48.62
1.845	2	5 1 1	49.36
1.841	3	-6 0 3	49.48
1.798	4	0 0 5 +	50.72
1.794	4	-4 0 5	50.86
1.791	5	-5 1 4 +	50.94
1.787	3	-6 1 1	51.06
1.764	7	-3 1 5 +	51.78
1.760	5	-2 2 4	51.92
1.753	3	-1 2 4	52.12
1.749	2	4 0 3	52.26
1.737	5	-6 1 3	52.66
1.725	1	1 3 0 +	53.06
1.715	4	0 3 1 +	53.38
1.711	3	-6 0 4	53.50
1.706	3	0 2 4	53.68
1.701	2	0 1 5	53.84
1.678	1	1 3 1 +	54.66

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.673	3	5 2 0	54.82
1.663	4	2 3 0 +	55.18
1.628	2	0 3 2	56.48
1.613	3	-2 3 2 +	57.04
1.607	3	1 1 5 +	57.30
1.599	3	3 1 4	57.58
1.594	3	6 1 1	57.78
1.583	2	1 3 2	58.24
1.573	1	3 3 0 +	58.62
1.569	2	-7 1 2	58.82
1.557	1	-6 0 5	59.32
1.553	2	7 0 0 +	59.46
1.543	2	-4 0 6	59.88
1.541	2	-5 2 4 +	59.98
1.529	1	-1 3 3	60.48
1.525	1	-3 2 5	60.68
1.507	2	4 0 4	61.50
1.496	1	2 1 5	61.96
1.493	2	-4 3 1	62.14
1.490	3	6 2 0 +	62.24
1.483	2	0 2 5	62.60
1.475	1	5 1 3 +	62.96
1.458	1	6 1 2	63.80
1.453	2	5 2 2	64.02
1.419	1	1 2 5	65.76
1.406	1	-2 3 4	66.44
1.384	1	3 1 5	67.64
1.380	2	-7 2 1 +	67.88
1.376	1	-8 1 3	68.08
1.373	1	-7 2 3	68.26
1.339	1	-6 2 5 +	70.26
1.313	2	6 2 2	71.84
1.310	2	-2 1 7	72.02
1.297	1	7 1 2	72.84
1.294	1	-1 4 1	73.04
1.287	1	-2 3 5	73.54
1.275	1	-9 0 3	74.34
1.271	1	-8 1 5	74.58
1.261	1	-8 2 2	75.32
1.252	1	-4 3 5	75.96

L-Cysteine, $\text{HSCH}_2\text{CH}(\text{NH}_2)\text{COOH}$ - continued

Calculated Pattern (Integrated)			
d (Å)	I	hkl	2θ (°) $\lambda = 1.54056 \text{ Å}$
10.87	38	1 0 0	8.12
8.99	4	0 0 1	9.83
8.41	1	-1 0 1	10.50
6.03	3	1 0 1	14.69
5.52	2	-2 0 1	16.04
5.44	11	2 0 0	16.29
4.74	42	-1 0 2	18.71
4.72	71	1 1 0	18.78
4.53	100	0 1 1	19.59
4.50	89	0 0 2	19.73
4.45	32	-1 1 1	19.94
4.21	15	-2 0 2	21.10
3.95	15	1 1 1	22.46
3.82	3	-3 0 1	23.24
3.801	15	-2 1 1	23.38
3.773	29	2 1 0	23.56
3.744	45	1 0 2	23.75
3.625	49	3 0 0	24.54
3.515	61	-1 1 2	25.32
3.423	31	-3 0 2	26.01
3.412	44	0 1 2	26.09
3.281	23	-2 1 2	27.16
3.227	67	2 1 1	27.62
3.168	5	-1 0 3	28.15
3.089	9	-3 1 1	28.88
3.087	10	-2 0 3	28.90
3.046	3	1 1 2	29.29
3.035	2	3 0 1	29.41
2.997	5	0 0 3	29.78
2.981	67	3 1 0	29.95
2.866	5	-3 1 2	31.19
2.805	1	-3 0 3	31.88
2.761	23	-4 0 2	32.40
2.719	59	4 0 0	32.92
2.711	17	-1 1 3	33.02
2.674	2	1 0 3	33.49
2.660	32	-2 1 3	33.67
2.626	6	3 1 1	34.11
2.620	9	0 2 0	34.20
2.612	9	2 1 2	34.30
2.602	3	0 1 3	34.44
2.547	11	1 2 0	35.21
2.515	5	0 2 1	35.66
2.502	4	-1 2 1	35.87
2.473	8	-3 1 3	36.30
2.456	17	3 0 2	36.56
2.443	9	-4 1 2	36.76
2.413	2	4 1 0	37.23
2.403	1	1 2 1	37.40
2.394	4	4 0 1	37.54

d (Å)	I	hkl	2θ (°) $\lambda = 1.54056 \text{ Å}$
2.382	21	1 1 3	37.74
2.370	10	-2 0 4	37.94
2.360	3	2 2 0	38.10
2.360	3	-1 0 4	38.10
2.293	1	-1 2 2	39.26
2.293	1	-5 0 1	39.27
2.273	7	-3 0 4	39.62
2.248	13	0 0 4	40.08
2.224	7	-2 2 2	40.53
2.224	1	3 1 2	40.53
2.222	15	-4 1 3	40.57
2.207	2	2 2 1	40.85
2.177	5	4 1 1	41.43
2.161	5	-3 2 1	41.76
2.159	2	-2 1 4	41.80
2.152	1	-1 1 4	41.95
2.147	4	1 2 2	42.06
2.123	3	2 1 3	42.54
2.121	5	-5 0 3	42.58
2.104	2	-4 0 4	42.96
2.100	2	-5 1 1	43.03
2.085	6	-3 1 4	43.36
2.084	1	-5 1 2	43.39
2.080	6	-3 2 2	43.46
2.066	2	0 1 4	43.79
2.048	1	4 0 2	44.19
2.019	1	-1 2 3	44.86
2.009	1	3 0 3	45.09
1.998	1	-2 2 3	45.36
1.983	4	3 2 1	45.71
1.977	17	2 2 2	45.86
1.973	1	0 2 3	45.97
1.971	2	5 0 1	46.00
1.966	1	-5 1 3	46.12
1.952	1	-4 1 4	46.48
1.937	1	-4 2 1	46.87
1.926	1	1 1 4	47.15
1.915	2	-3 2 3	47.44
1.908	9	4 1 2	47.63
1.901	8	-4 2 2	47.82
1.887	1	4 2 0	48.20
1.876	1	-1 0 5	48.49
1.876	1	3 1 3	48.49
1.872	1	2 0 4	48.60
1.871	3	1 2 3	48.61
1.845	2	5 1 1	49.35
1.841	3	-6 0 3	49.47
1.798	5	0 0 5	50.72
1.796	2	-6 1 2	50.78
1.795	1	-4 0 5	50.83

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.792	2	3 2 2	50.92
1.791	2	-5 1 4	50.94
1.791	2	-4 2 3	50.96
1.789	1	-2 1 5	51.01
1.787	1	-6 1 1	51.06
1.766	2	-1 1 5	51.72
1.764	9	-3 1 5	51.77
1.763	2	2 1 4	51.82
1.757	1	-2 2 4	51.99
1.753	3	-1 2 4	52.12
1.749	1	4 0 3	52.27
1.737	7	-6 1 3	52.66
1.725	1	-5 2 1	53.03
1.725	1	1 3 0	53.06
1.717	1	-3 2 4	53.31
1.716	2	-5 2 2	53.34
1.715	4	0 3 1	53.39
1.713	1	6 1 0	53.45
1.711	1	-6 0 4	53.50
1.706	4	0 2 4	53.68
1.701	1	0 1 5	53.85
1.680	1	3 0 4	54.59
1.678	1	1 3 1	54.66
1.673	4	5 2 0	54.81
1.665	1	-2 3 1	55.10
1.663	6	2 3 0	55.19
1.626	2	0 3 2	56.47
1.614	1	4 2 2	57.03
1.613	3	-2 3 2	57.04
1.612	1	-7 0 3	57.10
1.607	2	2 3 1	57.30
1.606	2	1 1 5	57.31
1.599	4	3 1 4	57.58
1.594	4	6 1 1	57.78
1.583	3	1 3 2	58.24
1.575	1	5 2 1	58.55
1.574	1	3 3 0	58.62
1.569	3	-7 1 2	58.82
1.557	2	-6 0 5	59.31
1.555	1	-1 0 6	59.38
1.553	2	7 0 0	59.45
1.544	2	-4 0 6	59.87
1.541	2	-5 2 4	59.97
1.539	1	-6 2 1	60.07
1.530	2	-1 3 3	60.48
1.524	1	-3 2 5	60.71
1.507	2	4 0 4	61.49
1.497	1	2 1 5	61.96
1.493	2	-4 3 1	62.12
1.491	2	6 2 0	62.23

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.489	2	7 1 0	62.29
1.483	2	0 2 5	62.60
1.476	1	-4 3 2	62.91
1.475	1	5 1 3	62.97
1.462	1	1 3 3	63.57
1.457	2	6 1 2	63.81
1.453	1	5 2 2	64.02
1.419	1	1 2 5	65.77
1.406	1	-2 3 4	66.44
1.384	1	3 1 5	67.65
1.380	1	-7 1 5	67.88
1.379	1	-7 2 1	67.89
1.376	1	-8 1 3	68.08
1.373	1	-7 2 3	68.26
1.348	1	-5 3 3	69.67
1.344	1	-4 0 7	69.94
1.339	1	7 0 2	70.23
1.338	2	-6 2 5	70.27
1.330	1	-4 2 6	70.79
1.313	2	6 2 2	71.84
1.310	2	-2 1 7	72.01
1.297	1	7 1 2	72.84
1.294	1	-1 4 1	73.04
1.287	1	-2 3 5	73.53
1.275	1	-9 0 3	74.35
1.271	1	-8 1 5	74.59
1.261	1	-8 2 2	75.32
1.252	1	-4 3 5	75.96

Structure

Hexagonal, $R\bar{3}m(166)$, $Z=3$. The structure was determined by Penfold and Taylor [1960].

Lattice parameters

$a=9.50(1)$, $c=4.82(1)$ Å [ibid.]

Density

(calculated) 2.19 g/cm^3

Thermal parameters

Isotropic [ibid.]

Atomic positions

In a disordered atomic arrangement, the 6 fluoride atoms and 12 water molecules were found to occupy one set of 36-fold positions, each site containing on the average ($\frac{1}{6}\text{F}^-$ and $\frac{1}{3}\text{O}^0$). The hydrogen positions were not determined [ibid.].

Polymorphism

Two kinds of white crystals precipitated together: the form "A", described here, and a form "B" which appeared to have a very similar structure with the c doubled [ibid.]

Scattering factors

Fe^{2+} [Thomas and Umeda, 1957]
 $(\frac{1}{6}\text{F}^- + \frac{1}{3}\text{O}^0)$ [Berghuis et al., 1955].

Scale factor

(integrated intensities) 3.406×10^4

Additional patterns

1. PDF card 22-626 [Ostrovskaya and Amirova, 1969]

Calculated Pattern (Peak heights)

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
4.75	100	1 1 0	18.66
4.16	57	1 0 1	21.36
3.13	5	0 2 1	28.50
2.74	1	3 0 0	32.62
2.61	35	2 1 1	34.30
2.374	1	2 2 0	37.86
2.080	5	2 0 2	43.48
2.062	1	1 3 1	43.86
1.905	12	1 2 2	47.70
1.892	9	4 0 1	48.06
1.795	5	4 1 0	50.82
1.758	5	3 2 1	51.98
1.657	8	3 1 2	55.40
1.583	2	3 3 0	58.22
1.564	1	0 4 2	59.00
1.557	1	0 5 1	59.30
1.522	2	1 1 3	60.82
1.486	2	2 3 2	62.44
1.480	2	2 4 1	62.74
1.413	1	5 1 1	66.08
1.386	2	0 3 3	67.52
1.371	1	6 0 0	68.36
1.331	1	2 2 3	70.74
1.317	2	5 2 0	71.56
1.214	1	1 6 1	78.76
1.197	1	1 4 3	80.08
1.192	1	1 0 4	80.48
1.142	1	3 5 1	84.84

Reference

- Berghuis, J., Haanapel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H., and Veenendaal, A. L. (1955). *Acta Cryst.* 8, 478.
 Ostrovskaya, T.V., and Amirova, S.A. (1969). *Zh. Neorgan. Khim.* 14, 1443. *Russ. J. Inorg. Chem.* (English transl.) 14, 755.
 Penfold, B.R., and Taylor, M.R. (1960). *Acta Cryst.* 13, 953.
 Thomas, L.H. and Umeda, K. (1957). *J. Chem. Phys.* 26, 293.

Iron fluoride hydrate, $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ - continued

Calculated Pattern (<i>Integrated</i>)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
4.75	100	1 1 0	18.67
4.16	60	1 0 1	21.35
3.13	5	0 2 1	28.50
2.74	1	3 0 0	32.63
2.61	42	2 1 1	34.29
2.375	1	2 2 0	37.85
2.079	6	2 0 2	43.48
2.062	1	1 3 1	43.86
1.905	15	1 2 2	47.70
1.892	11	4 0 1	48.05
1.795	7	4 1 0	50.81
1.758	7	3 2 1	51.99
1.657	11	3 1 2	55.40
1.583	2	3 3 0	58.22
1.565	2	0 4 2	58.99
1.557	1	0 5 1	59.29
1.522	3	1 1 3	60.81
1.486	3	2 3 2	62.45
1.480	3	2 4 1	62.74
1.413	2	5 1 1	66.08
1.386	3	0 3 3	67.51
1.371	2	6 0 0	68.35
1.331	2	2 2 3	70.74
1.317	3	5 2 0	71.56
1.307	1	4 2 2	72.25
1.302	1	4 3 1	72.53
1.214	2	1 6 1	78.75
1.197	2	1 4 3	80.09
1.192	1	1 0 4	80.49
1.142	2	3 5 1	84.84
1.128	1	3 3 3	86.16
1.019	1	5 2 3	98.25
.965	1	4 5 2	105.89
.944	1	8 1 1	109.32
.934	1	5 1 4	111.14
.926	1	4 6 1	112.55
.871	1	6 3 3	124.35
.812	1	9 1 2	143.10
.807	1	1 5 5	145.13
.799	1	9 2 1	148.96
.795	1	0 9 3	151.61
.785	1	3 4 5	157.76
.784	1	2 8 3	158.80

Lithium hydroxide hydrate, $\text{LiOH}\cdot\text{H}_2\text{O}$

Structure

Monoclinic, I2/m (12), $Z=4$. Pepinsky [1939] determined the structure and published his data in terms of the C2/m cell with $a=7.37\text{kX}$, $b=8.26\text{kX}$, $c=3.19\text{kX}$, and $\beta=110^\circ 18'$. Rabaud and Gay [1955] did further work, and Alcock [1971] refined their data to determine all the hydrogen positions.

Lattice parameters

$a=6.95$, $b=8.28$, $c=3.20\text{Å}$, $\beta=95.23^\circ$.

Density

(calculated) 1.53 g/cm^3

Thermal parameters

Isotropic: hydrogen(1): $B=12.3$; hydrogen(2): $B=14.0$ [Alcock, 1971]; lithium: $B=3.82$; oxygen(1): $B=2.87$ oxygen(2): $B=4.67$.

Atomic positions

Alcock [1971].

Scattering factors

Li^+ , O^0 [International Tables, 1962]

H^0 [McWeeny, 1951]

Scale factor

(integrated intensities) 0.1301×10^4

Additional patterns

1. PDF card 1-1062 [Dow Chemical Co., Midland, Michigan].

Reference

- Alcock, N.W. (1971). Acta Cryst. B27, 1682.
International Tables for X-ray Crystallography III 1962, pg. 202.
McWeeny, R. (1951). Acta Cryst. 4, 513.
Pepinsky, R. (1937). Z. Krist. 102A, 119.
Rabaud, H. and Gay, R. (1957). Bull. Soc. Franç. Minéral Crist. 80, 166.

Calculated Pattern (Peak heights)			
d (Å)	I	hkl	$2\theta(^\circ)$ $\lambda = 1.54056 \text{ Å}$
4.14	2	C 2 0	21.44
3.47	3	-2 0 0	25.68
2.97	66	0 1 1	30.02
2.80	24	1 0 1	31.94
2.66	100	-2 2 0	33.70
2.56	11	-1 3 0	34.96
2.43	45	-1 2 1	36.96
2.225	6	-3 1 0	40.50
2.167	3	2 1 1	41.64
2.086	1	C 3 1	43.34
2.070	6	0 4 0	43.70
1.958	8	-3 0 1	46.34
1.836	9	-2 3 1	49.60
1.777	3	-2 4 0	51.38
1.742	13	2 3 1	52.48
1.733	6	-4 0 0	52.78
1.664	3	1 4 1	55.14
1.646	1	3 2 1	55.80
1.611	1	-1 5 0	57.14
1.593	2	C 0 2	57.82
1.557	2	-1 1 2	59.32
1.500	2	-2 0 2	61.78
1.497	2	1 1 2	61.92
1.470	3	C 5 1	63.22
1.445	2	4 1 1	64.44
1.422	3	-3 4 1	65.58
1.380	1	C 6 0	67.86
1.374	2	-1 3 2 +	68.18
1.367	1	-5 1 0	68.58
1.353	1	-3 1 2	69.40
1.346	1	-3 5 0	69.82
1.326	1	2 2 2	71.02
1.254	1	-5 2 1 +	75.80
1.179	1	-4 2 2	81.56

Calculated Pattern (<i>Integrated</i>)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
4.14	2	0 2 0	21.45
3.47	3	-2 0 0	25.68
2.97	64	0 1 1	30.02
2.80	24	1 0 1	31.94
2.66	100	-2 2 0	33.70
2.56	11	-1 3 0	34.96
2.43	46	-1 2 1	36.96
2.225	6	-3 1 0	40.50
2.167	4	2 1 1	41.64
2.086	1	0 3 1	43.33
2.070	7	0 4 0	43.69
1.957	10	-3 0 1	46.35
1.837	11	-2 3 1	49.59
1.777	3	-2 4 0	51.37
1.742	16	2 3 1	52.49
1.733	7	-4 0 0	52.79
1.664	4	1 4 1	55.13
1.646	1	3 2 1	55.80
1.611	1	-1 5 0	57.14
1.593	3	0 0 2	57.82
1.557	2	-1 1 2	59.32
1.501	2	-2 0 2	61.77
1.498	2	1 1 2	61.91
1.469	4	0 5 1	63.23
1.445	3	4 1 1	64.45
1.422	4	-3 4 1	65.59
1.380	1	0 6 0	67.86
1.374	2	-1 3 2	68.18
1.374	1	-4 3 1	68.20
1.367	1	-5 1 0	68.58
1.353	1	-3 1 2	69.40
1.346	2	-3 5 0	69.82
1.326	2	2 2 2	71.02
1.254	1	-5 2 1	75.79
1.254	1	-1 6 1	75.81
1.239	1	-5 3 0	76.90
1.179	1	-4 2 2	81.57
1.121	1	1 5 2	86.82
1.098	1	4 5 1	89.09

Magnesium chloride (chloromagnesite), $MgCl_2$

Structure

Hexagonal, $R\bar{3}m$ (166), $Z=3$, isostructural with $CdCl_2$. The structure was determined by Pauling [1929].

Lattice parameters

$a=3.632(4)$, $c=17.795(16)\text{\AA}$ [Ferrari et al., 1963]

Density

(calculated) 3.540 g/cm^3

Thermal parameters

Isotropic, overall $B=2.0$

Scattering factors

Mg^{2+} , Cl^- [International Tables, 1962]

Scale factor

(integrated intensities) 1.022×10^4

Reference

Ferrari, A., Braibanti, A., and Bigliardi, G. (1963).

Acta Cryst. 16, 846.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938)

Ind. Eng. Chem. Anal. Ed. 10, 457.

International Tables for X-ray Crystallography III (1962), pg. 202.

Pauling, L. (1929). Proc. Nat'l. Acad. Sci. USA 15, 709.

Calculated Pattern (Peak heights)

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
5.93	24	0 0 3	14.92
3.097	13	1 0 1	28.80
2.966	53	0 1 2 +	30.10
2.569	100	1 0 4	34.90
2.356	5	0 1 5	38.16
1.977	3	1 0 7 +	45.86
1.816	45	1 1 0 +	50.20
1.737	3	1 1 3	52.66
1.567	1	0 2 1	58.90
1.549	7	1 1 6 +	59.64
1.483	11	0 2 4 +	62.60
1.439	1	2 0 5 +	64.74
1.338	1	1 1 9	70.32
1.284	4	2 0 8	73.72
1.178	2	1 2 2 +	81.64
1.148	8	2 1 4 +	84.24
1.048	5	1 2 8 +	94.56
.989	1	2 1 10	102.38
.908	1	2 2 0 +	116.06
.868	1	3 1 2 +	125.04
.856	3	1 3 4 +	128.24
.812	2	3 1 8 +	143.04
.783	1	1 3 10 +	159.06

Calculated Pattern (Integrated)

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
5.93	19	0 0 3	14.92
3.097	12	1 0 1	28.80
2.966	13	0 0 6	30.10
2.966	40	0 1 2	30.11
2.568	100	1 0 4	34.90
2.357	5	0 1 5	38.15
1.977	1	0 0 9	45.85
1.977	3	1 0 7	45.86
1.816	26	0 1 8	50.19
1.816	26	1 1 0	50.20
1.736	3	1 1 3	52.67
1.567	1	0 2 1	58.90
1.549	2	1 0 10	59.64
1.549	5	1 1 6	59.65
1.549	2	2 0 2	59.65
1.483	4	0 0 12	62.58
1.483	11	0 2 4	62.60
1.439	1	0 1 11	64.74
1.439	1	2 0 5	64.75
1.338	1	1 1 9	70.33
1.284	6	2 0 8	73.71
1.179	1	0 1 14	81.63
1.178	1	0 2 10	81.63
1.178	2	1 2 2	81.64
1.149	7	1 1 12	84.23
1.149	7	2 1 4	84.24
1.049	2	1 0 16	94.54
1.049	5	1 2 8	94.55
1.048	2	3 0 0	94.56
.989	1	2 1 10	102.37
.908	2	0 2 16	116.04
.908	2	2 2 0	116.06
.868	1	1 1 18	125.02
.868	1	1 2 14	125.03
.868	1	2 2 6	125.04
.868	1	3 1 2	125.05
.856	2	0 1 20	128.22
.856	2	3 0 12	128.25
.856	2	0 3 12	128.25
.856	3	1 3 4	128.26
.812	4	2 1 16	143.02
.812	4	3 1 8	143.04
.783	1	1 0 22	158.98
.783	2	1 3 10	159.06
.783	1	0 4 2	159.08

Additional patterns

1. PDF 3-0854 [Hanawalt et al., 1938]

Manganese oxide (partridgeite), α - Mn_2O_3 (revised)

Structure

Orthorhombic, $Pcab$ (61), $Z=16$. The structure was determined by Norrestam [1967] and confirmed by Geller [1971]. The structure had previously been reported as a cubic, C-type sesquioxide [Pauling and Shappell, 1930; Swanson et al., 1960].

Lattice parameters

$a=9.4161(3)$, $b=9.4237(3)$, $c=9.4051(3)\text{\AA}$ (published values: $9.4157(3)$, $9.4233(3)$, $9.4047(3)\text{\AA}$) [Geller, 1971]

Density

(calculated) 5.026 g/cm^3

Thermal parameters

Isotropic:

Manganese(1) $B=0.335$	oxygen(6) $B=0.641$
Manganese(2) $B=0.416$	oxygen(7) $B=0.684$
Manganese(3) $B=0.577$	oxygen(8) $B=0.606$
Manganese(4) $B=0.584$	oxygen(9) $B=0.517$
Manganese(5) $B=0.573$	oxygen(10) $B=0.629$
	oxygen(11) $B=0.598$

Atomic positions

Geller [1971]

Polymorphism

Above 35°C , α - Mn_2O_3 becomes cubic. (Substitution of less than one cation % Fe^{3+} for the Mn^{3+} ion makes the compound cubic, at room temperature.) [Geller, 1971]. The alpha form described here was called β - Mn_2O_3 by Morozov and Kuznetsov [1949]. A polymorph called γ - Mn_2O_3 was prepared by dehydration of $\text{Mn}_2\text{O}_3 \cdot \text{H}_2\text{O}$, and was somewhat unstable [Verwey and deBoer, 1936].

Scattering factors

Mn^{3+} [Cromer and Waber, 1965], corrected for dispersion [Cromer, 1965].

O^{2-} [Tokonami, 1965]

Scale factor

(integrated intensities) 54.67×10^4

Additional patterns

1. PDF card 10-69 [Swanson et al., 1960].

Calculated Pattern (Peak heights)			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
4.706	1	0 0 2 +	18.84
3.844	18	1 1 2 +	23.12
3.1379	<1	2 1 2 +	28.42
2.7185	100	2 2 2	32.92
2.5157	2	3 1 2 +	35.66
2.3540	11	0 4 0 +	38.20
2.2192	<1	4 1 1 +	40.62
2.1054	<1	2 4 0 +	42.92
2.0069	9	3 3 2 +	45.14
1.9210	1	2 2 4 +	47.28
1.8462	10	3 4 1 +	49.32
1.7191	2	5 1 2 +	53.24
1.6643	27	4 4 0 +	55.14
1.6143	2	3 3 4 +	57.00
1.5686	<1	0 0 6 +	58.82
1.5272	2	1 1 6 +	60.58
1.4887	<1	6 0 2 +	62.32
1.4524	4	5 1 4 +	64.06
1.4196	11	2 6 2 +	65.72
1.3883	3	6 1 3 +	67.40
1.3589	3	4 4 4	69.06
1.3314	<1	3 5 4 +	70.70
1.3052	<1	4 6 0 +	72.34
1.2814	1	1 7 2 +	73.90
1.2802	1	2 1 7 +	73.98
1.2585	<1	6 4 2 +	75.48
1.1956	<1	5 6 1 +	80.22
1.1772	1	0 8 0 +	81.74
1.1755	1	0 0 8	81.88
1.1591	1	8 1 1 +	83.30
1.1579	1	1 1 8 +	83.40
1.1419	<1	8 2 0 +	84.84
1.1406	<1	2 0 8 +	84.96
1.1252	1	6 5 3 +	86.40
1.1097	<1	2 8 2 +	87.92
1.1087	<1	2 2 8	88.02
1.0945	<1	1 3 8 +	89.46
1.0798	2	6 6 2 +	91.02

References

- Geller, S. (1971). Acta Cryst. B27, 821.
 Morozov, I.S. and Kuznetsov, V.G. (1949). Izvest. Akad. Nauk. SSSR Otdel. Khim. Nauk, No. 4, 343.
 Norrestam, R. (1967). Acta Chem. Scand. 21, 19.
 Pauling, L. and Shappell, M. D. (1930). Z. Krist. 75, 128.
 Tokonami, M. (1965). Acta Cryst. 19, 486.
 Swanson, H. E., Cook, M., Isaacs, T., and Evans, E.H. (1960). Nat'l. Bur. Std. U.S. Circ. 539, No. 9, 37.
 Verwey, E.G.W., and deBoer, J.H. (1936). Rec. trav. chim. 55, 531.

Manganese oxide (partridgeite), α Mn_2O_3 (revised) – continued

Calculated Pattern (<i>Integrated</i>)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
3.845	5	1 2 1	23.11
3.844	5	2 1 1	23.12
3.842	6	1 1 2	23.13
2.7179	100	2 2 2	32.93
2.3559	5	0 4 0	38.17
2.3540	5	4 0 0	38.20
2.3513	5	0 0 4	38.25
2.0078	4	3 3 2	45.12
2.0072	4	2 3 3	45.13
2.0069	4	3 2 3	45.14
1.8475	2	3 4 1	49.28
1.8471	2	4 3 1	49.29
1.8468	2	1 4 3	49.30
1.8460	2	4 1 3	49.33
1.8458	2	1 3 4	49.33
1.8454	2	3 1 4	49.34
1.6652	13	4 4 0	55.11
1.6642	13	0 4 4	55.14
1.6636	13	4 0 4	55.17
1.5286	1	1 6 1	60.52
1.5275	1	0 1 1	60.57
1.5258	1	1 1 6	60.64
1.4536	1	4 5 1	64.00
1.4533	1	5 4 1	64.01
1.4530	1	1 5 4	64.03
1.4524	1	1 4 5	64.06
1.4523	1	5 1 4	64.06
1.4519	1	4 1 5	64.08
1.4203	7	2 6 2	65.68
1.4195	7	6 2 2	65.73
1.4183	7	2 2 6	65.79
1.3892	1	3 6 1	67.35
1.3889	1	1 6 3	67.37
1.3885	1	6 3 1	67.39
1.3880	1	6 1 3	67.41
1.3873	1	1 3 6	67.46
1.3871	1	3 1 6	67.47
1.3589	4	4 4 4	69.06
1.2822	1	1 7 2	73.85
1.2814	1	7 2 1	73.90
1.2800	1	2 1 7	73.99
1.1780	1	0 8 0	81.67
1.1770	1	8 0 0	81.75
1.1756	1	0 0 8	81.87
1.1599	1	1 8 1	83.22
1.1590	1	8 1 1	83.30
1.1577	1	1 1 8	83.42
1.0804	2	6 6 2	90.95
1.0799	2	2 6 6	91.00
1.0795	2	6 2 6	91.04

Structure

Orthorhombic, Pbnm (62), Z=4. It is isostructural with goethite (α -FeOOH) and diaspore (α -AlOOH) [Gruner, 1947]. The groutite structure was determined by Collin and Lipscomb [1949] and refined by Glasser and Ingram [1968].

Lattice parameters

a=4.560, b=10.700, c=2.870(Å) [Glasser and Ingram, 1968]

Density

(calculated) 4.171 g/cm³

Thermal parameters

Isotropic [Glasser and Ingram, 1968]

Atomic positions

Glasser and Ingram [1968].

Polymorphism

MnOOH occurs also as two other minerals: manganite (γ form, monoclinic) and feitnechtite (β form, hexagonal).

Scattering factors

Mn³⁺ [International Tables, 1962]

O²⁻ [Suzuki, 1960]

Scale factor

(integrated intensities) 0.7057×10^4

Additional patterns

1. PDF card 12-733 [Thompson, R.M., Univ. of British Columbia, Vancouver, British Columbia, Canada.]

Reference

Collin, R.L. and Lipscomb, W.N. (1949). Acta Cryst. 2, 104.

Glasser, L.S.D. and Ingram, L. (1968). Acta Cryst. B24, 1233.

International Tables for X-ray Crystallography III 1962, 210.

Suzuki, T. (1960). Acta Cryst. 13, 279.

Calculated Pattern (Peak heights)

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
5.35	9	0 2 0	16.56
4.20	100	1 1 0	21.16
3.471	10	1 2 0	25.64
2.810	34	1 3 0	31.82
2.674	29	0 4 0	33.48
2.529	13	0 2 1	35.46
2.429	4	1 0 1	36.98
2.368	48	1 1 1	37.96
2.308	17	1 4 0	39.00
2.280	2	2 0 0	39.50
2.230	2	2 1 0	40.42
2.212	7	1 2 1	40.76
2.008	5	1 3 1	45.12
1.957	3	0 4 1	46.36
1.937	4	1 5 0	46.86
1.798	3	1 4 1	50.72
1.783	2	0 6 0	51.18
1.761	9	2 1 1	51.88
1.735	6	2 4 0	52.70
1.693	26	2 2 1	54.12
1.606	18	1 5 1	57.34
1.596	7	2 3 1	57.70
1.560	3	2 5 0	59.16
1.515	9	0 6 1	61.14
1.485	1	2 4 1	62.50
1.462	4	3 2 0	63.58
1.449	4	1 7 0	64.22
1.435	6	0 0 2	64.94
1.404	1	2 6 0	66.52
1.398	3	3 3 0	66.86
1.358	3	1 1 2	69.12
1.343	3	3 0 1	69.98
1.333	1	3 1 1	70.62
1.326	1	1 2 2	71.02
1.303	1	3 2 1	72.50
1.278	4	1 3 2	74.14
1.264	3	0 4 2	75.06
1.262	3	2 6 1	75.26
1.257	2	3 3 1	75.58
1.218	1	1 4 2	78.42
1.215	1	2 0 2	78.72
1.212	2	0 8 1	78.90
1.200	3	3 4 1	79.84
1.157	1	3 6 0	83.50
1.154	3	2 8 0 +	83.78
1.133	2	4 1 0	85.62
1.106	2	2 4 2	88.30
1.078	1	3 7 0	91.24
1.073	1	3 6 1	91.76
1.070	2	2 8 1 +	92.06

Manganese oxide hydroxide, groutite, alpha MnOOH – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.068	3	1 9 1	92.34
1.056	1	2 5 2	93.66
1.054	1	2 9 0	93.90
1.024	1	3 2 2	97.54
1.020	2	1 7 2	98.12
1.016	1	4 3 1	98.66
1.006	1	4 5 0	99.92
1.004	1	2 6 2	100.24
1.003	1	0 10 1	100.40
1.001	2	3 3 2	100.56
.951	1	1 11 0	108.14
.948	1	3 8 1	108.72
.933	1	1 1 3	111.34
.901	1	3 6 2	117.58
.899	2	2 8 2 +	117.90
.890	2	4 1 2	119.98
.871	4	4 7 1 +	124.42
.869	2	5 0 1	124.96
.866	1	4 3 2	125.64
.862	1	3 7 2	126.70
.858	2	1 5 3 +	127.80
.856	1	2 3 3	128.20
.854	1	2 11 1	128.78
.852	1	0 12 1	129.54
.850	1	2 9 2	130.10
.843	1	0 6 3	132.04
.827	1	5 4 1	137.44
.824	1	4 5 2	138.46
.823	1	3 8 2	138.86

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
5.35	9	0 2 0	16.56
4.19	100	1 1 0	21.16
3.470	11	1 2 0	25.65
2.809	40	1 3 0	31.83
2.675	34	0 4 0	33.47
2.529	15	0 2 1	35.46
2.429	5	1 0 1	36.98
2.369	58	1 1 1	37.95
2.307	21	1 4 0	39.00
2.280	2	2 0 0	39.49
2.230	2	2 1 0	40.42
2.212	8	1 2 1	40.76
2.008	6	1 3 1	45.12
1.957	3	0 4 1	46.36
1.937	5	1 5 0	46.86
1.921	1	2 3 0	47.28
1.798	4	1 4 1	50.73
1.783	2	0 6 0	51.18
1.761	13	2 1 1	51.88
1.735	9	2 4 0	52.71
1.693	38	2 2 1	54.11
1.606	26	1 5 1	57.33
1.596	9	2 3 1	57.70
1.560	5	2 5 0	59.16
1.515	13	0 6 1	61.13
1.485	2	2 4 1	62.50
1.462	6	3 2 0	63.58
1.449	7	1 7 0	64.21
1.435	9	0 0 2	64.93
1.405	2	2 6 0	66.51
1.398	4	3 3 0	66.85
1.358	6	1 1 2	69.13
1.343	4	3 0 1	69.98
1.333	2	3 1 1	70.61
1.326	1	1 2 2	71.02
1.303	1	3 2 1	72.49
1.278	6	1 3 2	74.13
1.265	5	0 4 2	75.05
1.262	2	2 6 1	75.25
1.257	3	3 3 1	75.58
1.219	3	1 4 2	78.41
1.214	1	2 0 2	78.73
1.212	3	0 8 1	78.90
1.200	5	3 4 1	79.84
1.161	1	2 7 1	83.12
1.157	2	3 6 0	83.50
1.154	3	2 8 0	83.78
1.153	1	1 5 2	83.83
1.138	1	3 5 1	85.23
1.134	4	4 1 0	85.61

Manganese oxide hydroxide, groutite, alpha MnOOH – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.118	1	0 6 2	87.10
1.106	3	2 4 2	88.30
1.086	1	4 3 0	90.37
1.078	1	3 7 0	91.23
1.073	2	3 6 1	91.77
1.070	1	2 8 1	92.05
1.070	1	0 10 0	92.09
1.068	5	1 9 1	92.33
1.056	2	2 5 2	93.65
1.054	2	2 9 0	93.89
1.024	3	3 2 2	97.55
1.020	4	1 7 2	98.12
1.016	2	4 3 1	98.65
1.006	2	4 5 0	99.92
1.004	1	2 6 2	100.23
1.003	2	0 10 1	100.40
1.001	3	3 3 2	100.55
.979	1	1 10 1	103.75
.969	1	2 10 0	105.35
.951	2	1 11 0	108.13
.948	1	3 8 1	108.73
.942	1	0 2 3	109.76
.933	3	1 1 3	111.35
.901	2	3 6 2	117.58
.899	4	2 8 2	117.90
.899	2	5 2 0	117.92
.890	2	3 9 1	119.82
.890	5	4 1 2	119.98
.879	1	2 1 3	122.36
.871	7	4 7 1	124.40
.870	5	2 2 3	124.49
.869	2	5 0 1	124.80
.866	2	4 3 2	125.64
.862	2	3 7 2	126.71
.858	1	0 10 2	127.79
.858	5	1 5 3	127.79
.856	2	2 3 3	128.18
.854	1	2 11 1	128.79
.852	2	0 12 1	129.54
.850	3	2 9 2	130.10
.843	3	0 6 3	132.05
.837	2	3 10 1	133.96
.827	5	5 4 1	137.44
.824	4	4 5 2	138.46
.823	1	4 9 0	138.82
.823	2	3 8 2	138.87

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (alpha HMX) $C_4H_8N_8O_8$

Structure

Orthorhombic, Fdd2 (43), Z=8. The structure was determined by Cady et al. [1963].

Lattice parameters

a=15.14, b=23.89, c=5.913Å [ibid.]

Density

(calculated) 1.839 g/cm³

Thermal parameters

Isotropic: carbon(1) B=2.731, carbon(2) B=2.641, nitrogen(1) B=2.093, nitrogen(2) B=2.374, nitrogen(3) B=2.992, nitrogen(4) B=2.900, oxygen(1) B=3.587, oxygen(2) B=4.234, oxygen(3) B=3.003, oxygen(4) B=3.658, hydrogen(3) =3.60, hydrogens (1), (2), and (4) B=0.0

Atomic positions

Erratum: in Cady et al. [op. cit.], $y_{N(1)}$ should be -0.0599 in order to derive the structure factors they give.

Polymorphism

There are 4 known polymorphic forms. The alpha modification described here is stable in the range 103 to 162 °C. [Cady, et al., 1963]

Scattering factors

C⁰, H⁰, N⁰, O⁰ [International Tables, 1962]

Scale factor

(integrated intensities) 26.64 x 10⁴

Reference

Cady, H.H., Larson, A.C., and Cromer, D.T. (1963). Acta Cryst. 16, 617.
International Tables for X-ray Crystallography III (1962). 202.

Calculated Pattern (<i>Peak heights</i>)			
<i>d</i> (Å)	<i>I</i>	<i>hkl</i>	<i>2θ</i> (°) $\lambda = 1.54056 \text{ Å}$
6.39	1	2 2 0	13.84
5.97	31	0 4 0	14.82
5.37	100	1 1 1	16.50
4.53	34	1 3 1	19.58
3.79	12	4 0 0 +	23.48
3.61	45	1 5 1 +	24.64
3.52	50	2 6 0	25.26
3.46	17	3 3 1	25.74
2.986	17	0 8 0 +	29.90
2.901	7	1 7 1	30.80
2.870	11	0 2 2	31.14
2.754	34	2 0 2	32.48
2.746	23	4 6 0	32.58
2.677	5	5 1 1	33.44
2.550	4	3 7 1 +	35.16
2.501	1	2 4 2	35.88
2.469	6	6 2 0	36.36
2.391	2	1 9 1	37.58
2.373	8	0 6 2	37.88
2.325	3	0 4 0 +	38.70
2.287	13	4 2 2	39.36
2.281	8	2 10 0	39.48
2.265	3	2 6 2	39.76
2.183	4	3 9 1	41.32
2.170	3	4 4 2	41.58
2.115	1	5 7 1	42.72
2.024	1	7 1 1	44.74
2.021	2	1 11 1	44.82
1.991	1	0 12 0	45.52
1.968	1	7 3 1	46.08
1.948	3	1 1 3	46.58
1.926	2	2 12 0	47.16
1.898	2	1 3 3	47.88
1.892	2	5 9 1	48.06
1.809	1	1 5 3	50.40
1.804	1	8 4 0	50.54
1.743	1	1 13 1	52.44
1.714	1	3 5 3	53.42
1.691	1	5 11 1	54.18
1.658	1	3 13 1	55.38
1.614	3	2 12 2 +	57.02
1.580	1	8 2 2	58.36
1.540	2	8 4 2	60.02
1.484	1	7 11 1	62.56

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (alpha HMX) $C_4H_8N_8O_8$ - continued

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
6.39	1	2 2 0	13.84
5.97	30	0 4 0	14.82
5.37	100	1 1 1	16.50
4.53	35	1 3 1	19.58
3.79	4	3 1 1	23.45
3.78	10	4 0 0	23.48
3.61	48	1 5 1	24.65
3.61	3	4 2 0	24.65
3.52	56	2 6 0	25.25
3.46	18	3 3 1	25.74
2.993	4	3 5 1	29.83
2.986	18	0 8 0	29.90
2.901	8	1 7 1	30.80
2.870	13	0 2 2	31.14
2.754	40	2 0 2	32.48
2.743	8	4 6 0	32.61
2.684	1	2 2 2	33.36
2.678	5	5 1 1	33.43
2.553	1	5 3 1	35.12
2.551	4	3 7 1	35.16
2.501	1	2 4 2	35.88
2.469	7	6 2 0	36.36
2.391	3	1 9 1	37.58
2.374	10	0 6 2	37.87
2.347	4	5 5 1	38.31
2.344	1	4 8 0	38.36
2.324	4	6 4 0	38.71
2.287	17	4 2 2	39.37
2.278	3	2 10 0	39.52
2.265	3	2 6 2	39.76
2.183	5	3 9 1	41.32
2.171	4	4 4 2	41.57
2.115	1	5 7 1	42.71
2.024	1	7 1 1	44.74
2.020	1	1 11 1	44.82
1.991	2	0 12 0	45.53
1.968	1	7 3 1	46.08
1.948	4	1 1 3	46.58
1.925	2	2 12 0	47.17
1.898	2	1 3 3	47.88
1.891	2	5 9 1	48.07
1.809	1	1 5 3	50.40
1.804	1	8 4 0	50.55
1.762	1	4 12 0	51.85
1.743	1	1 13 1	52.45
1.714	2	3 5 3	53.42
1.691	1	5 11 1	54.19
1.658	1	3 13 1	55.38
1.648	1	5 1 3	55.73
1.615	2	6 8 2	56.99

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.614	1	9 1 1	57.00
1.613	2	2 12 2	57.03
1.586	1	9 3 1	58.13
1.580	1	8 2 2	58.36
1.540	3	8 4 2	60.02
1.518	1	5 13 1	60.97
1.484	1	7 11 1	62.56
1.440	1	2 2 4	64.66
1.377	1	4 0 4	68.03
1.320	1	3 17 1	71.42

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (beta HMX) $C_4H_8N_8O_8$

Structure

Monoclinic, $P2_1/n$ (14), $Z=2$. The structure was determined first by Eiland and Pepinsky [1955]. Cady, Larson, and Cromer [1963] used Eiland's and Pepinsky's data and did a least squares refinement with anisotropic temperature factors, but did not determine the hydrogen positions. Choi and Boutin [1970] collected new 3-dimensional data from neutron diffraction analysis and re-fined parameters for all atoms including hydrogen.

Lattice parameters

$a=6.54$, $b=11.05$, $c=7.37\text{\AA}$, $\beta=102.8^\circ$ [Eiland and Pepinsky, 1955]

Density

(calculated) 1.89 g/cm^3

Thermal parameters

Isotropic: hydrogen(1): $B=2.892$; hydrogen(2): $B=2.726$; hydrogen(3): $B=2.790$; hydrogen(4): $B=3.686$ [Choi and Boutin, 1970]. Nitrogen(1): $B=1.616$; nitrogen(2): $B=1.468$; nitrogen(3): $B=1.361$; nitrogen(4): $B=1.676$; oxygen(1): $B=2.282$; oxygen(2): $B=2.769$; oxygen(3): $B=3.063$; oxygen(4): $B=2.523$; carbon(1): $B=1.294$; carbon(2): $B=1.600$.

Atomic positions

Choi and Boutin [1970]

Polymorphism

There are 4 known polymorphic forms. The beta modification described here is the stable form at room temperature [Cady et al., 1963].

Scattering factors

H^0 , O^0 , N^0 , C^0 [International Tables, 1962].

Scale factor

(Integrated intensities) 1.303×10^4

Additional patterns

1. PDF card 3-0225 [Soldate and Noyes, 1947]

Reference

Cady, H.H., Larson, A.C., and Cromer, D.T. (1963). Acta Cryst. **16**, 617.
Choi, C.S. and Boutin, H.P. (1970). Acta Cryst. **B26**, 1235.
Eiland, P.F. and Pepinsky, R. (1955). Z. Krist. **106**, 18.
International Tables for X-ray Crystallography III (1962), pg. 202.
Soldate, A.M. and Noyes, R.M. (1947). Anal. Chem. **19**, 442.

Calculated Pattern (Peak heights)			
d (Å)	I	hkl	$2\theta(^\circ)$ $\lambda = 1.54056\text{ \AA}$
6.02	39	0 1 1	14.70
5.52	40	1 1 0 +	16.04
5.40	2	-1 0 1	16.40
4.85	11	-1 1 1	18.26
4.32	100	1 0 1	20.56
4.02	8	1 1 1	22.08
3.86	53	-1 2 1	23.00
3.59	1	0 0 2	24.76
3.42	7	0 1 2	26.06
3.40	23	1 2 1	26.18
3.32	9	-1 1 2	26.84
3.28	28	0 3 1	27.18
3.19	12	1 3 0 +	27.96
3.06	13	-2 1 1 +	29.12
3.04	6	-1 3 1	29.32
3.01	33	0 2 2	29.64
2.94	4	-1 2 2	30.34
2.80	77	1 3 1	31.92
2.76	7	0 4 0 +	32.38
2.70	3	-2 0 2	33.14
2.62	1	2 1 1	34.16
2.57	1	0 3 2	34.86
2.53	4	1 4 0	35.38
2.46	2	-1 4 1	36.50
2.43	7	-2 2 2 +	37.02
2.41	8	2 3 0 +	37.26
2.26	3	1 3 2	39.78
2.22	1	-1 2 3	40.56
2.197	2	0 2 3	41.04
2.190	8	0 4 2	41.18
2.178	4	-2 3 2 +	41.42
2.158	2	2 0 2	41.82
2.133	4	-3 1 1	42.34
2.119	2	-2 1 3 +	42.64
2.113	2	0 5 1	42.76
2.088	5	2 4 0 +	43.30
2.027	1	-1 3 3	44.68
2.010	3	2 2 2 +	45.06
1.984	2	3 2 0	45.70
1.958	2	1 2 3	46.32
1.926	2	3 0 1	47.16
1.913	1	-3 2 2	47.50
1.897	2	3 1 1	47.92
1.883	1	0 5 2	48.30
1.872	2	-3 3 1	48.60
1.862	3	2 3 2 +	48.86
1.842	1	0 6 0	49.44
1.817	2	-2 5 1	50.18
1.810	1	0 4 3	50.38
1.801	4	-3 0 3	50.64

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.796	4	0 0 4	50.78
1.769	1	1 6 0	51.62
1.739	1	-2 0 4	52.58
1.710	1	2 5 1	53.54
1.685	1	3 4 0	54.42
1.669	2	1 4 3	54.96
1.659	1	-2 2 4	55.34
1.627	1	-1 6 2	56.50
1.615	1	0 3 4	56.98
1.594	1	-4 0 2	57.78
1.578	1	-4 1 2	58.44
1.573	1	-2 3 4	58.64
1.550	3	1 6 2 +	59.60
1.521	1	2 6 1	60.84
1.467	1	-1 6 3	63.34

Calculated Pattern (Integrated)

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
6.02	36	0 1 1	14.69
5.52	14	0 2 0	16.03
5.52	24	1 1 0	16.03
5.40	1	-1 0 1	16.39
4.85	11	-1 1 1	18.26
4.32	100	1 0 1	20.55
4.02	9	1 1 1	22.09
3.86	57	-1 2 1	23.00
3.59	1	0 0 2	24.76
3.42	6	0 1 2	26.05
3.40	24	1 2 1	26.17
3.32	10	-1 1 2	26.85
3.28	30	0 3 1	27.18
3.19	8	1 3 0	27.95
3.19	5	2 0 0	27.96
3.06	10	-2 1 1	29.12
3.06	4	2 1 0	29.13
3.04	5	-1 3 1	29.32
3.01	38	0 2 2	29.63
2.94	5	-1 2 2	30.34
2.80	92	1 3 1	31.91
2.76	5	0 4 0	32.38
2.76	2	2 2 0	32.39
2.70	4	-2 0 2	33.14
2.62	1	2 1 1	34.15
2.57	1	0 3 2	34.85
2.53	4	1 4 0	35.38
2.46	2	-1 4 1	36.50
2.43	2	-1 0 3	37.01
2.43	7	-2 2 2	37.01
2.41	1	-2 3 1	37.27
2.41	9	2 3 0	37.27

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.26	4	1 3 2	39.79
2.22	1	-1 2 3	40.56
2.198	2	0 2 3	41.03
2.190	9	0 4 2	41.18
2.178	4	-2 3 2	41.42
2.178	1	2 3 1	41.43
2.159	2	2 0 2	41.81
2.133	5	-3 1 1	42.34
2.119	1	-2 1 3	42.62
2.119	1	2 1 2	42.64
2.112	1	0 5 1	42.77
2.088	1	-2 4 1	43.30
2.088	4	2 4 0	43.30
2.027	1	-1 3 3	44.68
2.011	4	2 2 2	45.05
2.008	2	0 3 3	45.11
1.984	2	3 2 0	45.70
1.959	2	1 2 3	46.32
1.925	2	3 0 1	47.17
1.913	1	-3 2 2	47.50
1.897	3	3 1 1	47.92
1.882	1	0 5 2	48.31
1.872	3	-3 3 1	48.59
1.863	1	-2 3 3	48.85
1.862	3	2 3 2	48.86
1.842	2	0 6 0	49.45
1.816	1	-2 5 1	50.18
1.810	1	0 4 3	50.38
1.801	5	-3 0 3	50.65
1.797	2	0 0 4	50.77
1.769	2	1 6 0	51.61
1.743	1	-1 6 1	52.45
1.739	1	-2 0 4	52.58
1.710	1	2 5 1	53.54
1.685	1	3 4 0	54.42
1.669	3	1 4 3	54.97
1.659	1	-2 2 4	55.33
1.628	2	-1 6 2	56.49
1.615	1	0 3 4	56.98
1.594	1	-4 0 2	57.78
1.578	1	-4 1 2	58.43
1.573	1	-2 3 4	58.65
1.550	3	1 6 2	59.60
1.550	2	-3 5 1	59.61
1.522	1	2 6 1	60.83
1.467	2	-1 6 3	63.34
1.463	1	-4 3 2	63.53
1.452	1	3 5 1	64.09
1.401	2	2 6 2	66.70
1.354	1	-3 4 4	69.37

Potassium zinc bromide hydrate, $\text{KZnBr}_3 \cdot 2\text{H}_2\text{O}$

Structure

Orthorhombic, $\text{P2}_1\text{2}_1\text{2}_1$ (19), $Z=4$. The structure was determined by Holinski [1967].

Lattice parameters

$a=9.327(2)$, $b=13.067(4)$, $c=6.786(2)\text{\AA}$ [ibid]

Density

(calculated) 3.053 g/cm^3

Thermal parameters

Isotropic: bromine(1): $B=2.86$; bromine(2): $B=2.97$
bromine(3): $B=2.86$; zinc: $B=2.28$; potassium: $B=3.51$
water(1): $B=2.58$; water(2): $B=3.31$.

Atomic positions

To conform to the symmetry arrangements used in the International Tables I [1952], the values for the x parameters were replaced by $-x$. The value for $x_{\text{Br}(1)}$ should be -0.0129 in order to derive structure factors given by Holinski [op. cit.].

Scattering factors

O^0 , K^+ , Zn^{2+} [International Tables, 1962]
 Br^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 12.89×10^4

Reference

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
Holinski, R. (1967). Dissertation, Technischen Hochschule, 3392 Clausthal-Zellerfeld, W. Germany.

Calculated Pattern (Peak heights)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
7.58	6	1 1 0	11.66
6.53	18	0 2 0	13.54
6.02	14	0 1 1	14.70
5.49	47	1 0 1	16.14
5.35	11	1 2 0	16.56
5.06	13	1 1 1	17.52
4.706	21	0 2 1	18.84
4.392	1	2 1 0	20.20
4.203	4	1 2 1	21.12
3.844	32	2 0 1	23.12
3.795	2	2 2 0	23.42
3.687	5	2 1 1	24.12
3.666	4	0 3 1	24.26
3.411	63	1 3 1	26.10
3.312	5	2 2 1	26.90
3.283	13	0 1 2	27.14
3.184	100	1 0 2 +	28.00
3.097	5	1 1 2	28.80
3.089	3	1 4 0	28.88
3.023	2	3 1 0	29.52
2.944	1	0 4 1	30.34
2.882	48	2 3 1	31.00
2.826	28	3 0 1	31.64
2.763	2	3 1 1	32.38
2.743	1	2 0 2	32.62
2.685	7	2 1 2	33.34
2.676	5	2 4 0	33.46
2.595	2	3 2 1	34.54
2.573	14	1 3 2	34.84
2.489	3	2 4 1	36.06
2.371	4	3 3 1	37.92
2.360	1	1 5 1	38.10
2.321	3	2 3 2	38.76
2.292	3	3 0 2	39.28
2.285	2	1 4 2	39.40
2.252	2	3 4 0	40.00
2.205	6	4 0 1	40.90
2.198	5	1 0 3	41.02
2.178	20	0 6 0 +	41.42
2.171	12	1 1 3	41.56
2.161	3	2 5 1 +	41.76
2.138	2	3 4 1 +	42.24
2.083	1	1 2 3	43.40
2.071	1	0 5 2	43.68
2.055	10	4 3 0	44.02
2.035	10	2 0 3	44.48
2.028	30	3 3 2	44.64
2.024	20	1 6 1 +	44.74
2.008	4	0 3 3 +	45.12
2.002	3	3 5 0	45.26

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.967	8	4 3 1	46.10
1.963	5	1 3 3	46.22
1.943	3	2 2 3	46.70
1.919	1	3 5 1	47.34
1.901	1	4 1 2	47.80
1.895	6	2 6 1 +	47.98
1.844	11	2 3 3 +	49.38
1.833	1	0 6 2	49.70
1.828	2	4 4 1 +	49.84
1.811	1	3 1 3	50.34
1.798	14	1 6 2 +	50.72
1.767	2	1 7 1	51.68
1.758	1	4 3 2	51.96
1.740	1	4 5 0	52.56
1.734	2	5 2 1	52.74
1.725	7	3 6 1 +	53.04
1.697	5	0 0 4	54.00
1.686	2	4 5 1 +	54.38
1.682	2	0 1 4	54.50
1.669	1	1 0 4	54.98
1.663	11	5 3 1	55.20
1.658	6	4 4 2 +	55.38
1.635	2	0 7 2 +	56.20
1.624	3	4 0 3	56.64
1.611	1	1 7 2	57.14
1.609	1	1 8 0	57.20
1.606	1	2 5 3	57.32
1.588	1	0 8 1	58.04
1.579	1	3 6 2	58.40
1.575	2	5 4 1 +	58.54
1.566	1	1 8 1	58.94
1.559	1	1 3 4	59.24
1.555	3	6 0 0	59.40
1.549	3	4 6 1 +	59.62
1.530	1	5 3 2	60.44
1.521	3	4 3 3	60.84
1.518	2	5 5 0	61.00
1.497	3	2 3 4 +	61.92
1.487	3	2 6 3	62.40
1.462	1	5 4 2	63.60
1.454	1	4 4 3 +	63.98
1.431	1	6 3 1 +	65.12
1.423	1	0 5 4	65.54
1.409	1	3 3 4	66.28
1.404	2	1 9 1 +	66.56
1.386	2	2 9 0 +	67.50
1.367	2	5 3 3	68.62
1.358	1	2 9 1	69.10
1.355	1	3 4 4	69.30
1.338	3	0 6 4	70.28

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
7.59	7	1 1 0	11.65
6.53	22	0 2 0	13.54
6.02	17	0 1 1	14.70
5.49	59	1 0 1	16.14
5.35	14	1 2 0	16.55
5.06	16	1 1 1	17.51
4.707	27	0 2 1	18.84
4.392	1	2 1 0	20.20
4.202	5	1 2 1	21.13
3.843	45	2 0 1	23.12
3.796	1	2 2 0	23.42
3.687	6	2 1 1	24.12
3.666	5	0 3 1	24.26
3.412	91	1 3 1	26.10
3.393	4	0 0 2	26.24
3.313	6	2 2 1	26.89
3.284	19	0 1 2	27.13
3.189	100	1 0 2	27.96
3.183	87	2 3 0	28.01
3.098	7	1 1 2	28.80
3.083	1	1 4 0	28.94
3.025	3	3 1 0	29.51
2.943	2	0 4 1	30.34
2.882	75	2 3 1	31.01
2.866	3	1 2 2	31.19
2.826	46	3 0 1	31.63
2.763	2	3 1 1	32.38
2.744	2	2 0 2	32.61
2.685	10	2 1 2	33.34
2.676	4	2 4 0	33.46
2.594	3	3 2 1	34.55
2.573	22	1 3 2	34.84
2.530	1	2 2 2	35.46
2.489	5	2 4 1	36.05
2.371	6	3 3 1	37.92
2.359	2	1 5 1	38.11
2.321	4	2 3 2	38.76
2.292	4	3 0 2	39.27
2.282	1	1 4 2	39.46
2.252	3	3 4 0	40.00
2.229	1	0 1 3	40.44
2.205	10	4 0 1	40.89
2.198	2	1 0 3	41.02
2.178	34	0 6 0	41.43
2.174	1	4 1 1	41.49
2.168	1	1 1 3	41.63
2.163	1	3 2 2	41.72
2.161	3	2 5 1	41.76
2.138	1	0 2 3	42.24
2.137	3	3 4 1	42.25

Potassium zinc bromide hydrate, $\text{KZnBr}_3 \cdot 2\text{H}_2\text{O}$ - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.089	1	4 2 1	43.27
2.083	2	1 2 3	43.39
2.070	1	0 5 2	43.68
2.056	17	4 3 0	44.01
2.035	13	2 0 3	44.48
2.028	48	3 3 2	44.63
2.024	6	1 6 1	44.73
2.021	1	1 5 2	44.80
2.011	2	2 1 3	45.04
2.007	6	0 3 3	45.13
2.001	1	3 5 0	45.29
1.967	13	4 3 1	46.10
1.963	2	1 3 3	46.22
1.943	6	2 2 3	46.71
1.919	2	3 5 1	47.33
1.901	2	4 1 2	47.80
1.898	1	4 4 0	47.89
1.895	8	2 6 1	47.97
1.892	6	2 5 2	48.04
1.876	1	3 4 2	48.47
1.847	1	5 1 0	49.31
1.844	19	2 3 3	49.39
1.833	1	0 6 2	49.70
1.830	1	1 7 0	49.77
1.829	1	3 0 3	49.81
1.828	2	4 4 1	49.85
1.811	1	3 1 3	50.33
1.800	2	0 7 1	50.68
1.799	4	5 0 1	50.71
1.798	22	1 6 2	50.72
1.767	3	1 7 1	51.68
1.758	1	4 3 2	51.97
1.740	1	4 5 0	52.56
1.734	2	5 2 1	52.74
1.727	5	2 4 3	52.96
1.725	11	3 6 1	53.04
1.723	3	3 5 2	53.10
1.706	1	2 6 2	53.69
1.697	10	0 0 4	54.01
1.686	1	3 3 3	54.36
1.685	1	4 5 1	54.39
1.682	1	0 1 4	54.50
1.669	2	1 0 4	54.97
1.662	21	5 3 1	55.20
1.656	1	4 4 2	55.43
1.656	1	1 1 4	55.45
1.636	3	0 7 2	56.19
1.635	1	5 0 2	56.23
1.633	1	0 8 0	56.27
1.624	6	4 0 3	56.65

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.611	1	1 7 2	57.13
1.609	1	1 8 0	57.21
1.606	1	2 5 3	57.33
1.588	2	0 8 1	58.03
1.579	2	3 6 2	58.40
1.576	1	4 2 3	58.53
1.576	2	5 4 1	58.53
1.565	1	1 8 1	58.95
1.559	1	1 3 4	59.24
1.554	5	6 0 0	59.41
1.550	3	4 6 1	59.62
1.549	1	2 2 4	59.65
1.548	2	4 5 2	59.67
1.547	1	1 6 3	59.72
1.530	2	5 3 2	60.44
1.521	6	4 3 3	60.84
1.518	1	5 5 0	60.97
1.499	2	3 5 3	61.86
1.497	6	2 3 4	61.93
1.487	6	2 6 3	62.40
1.462	2	5 4 2	63.60
1.454	1	4 4 3	63.98
1.454	1	1 8 2	63.99
1.433	1	2 4 4	65.04
1.431	2	6 3 1	65.13
1.423	1	0 5 4	65.55
1.409	2	3 3 4	66.27
1.404	2	1 9 1	66.57
1.403	1	2 8 2	66.57
1.387	2	5 6 1	67.48
1.386	2	2 9 0	67.51
1.376	1	2 7 3	68.10
1.367	3	5 3 3	68.62
1.358	3	2 9 1	69.10
1.355	2	3 4 4	69.28
1.343	1	1 0 5	69.99
1.338	6	0 6 4	70.28
1.325	1	1 6 4	71.10
1.311	1	1 8 3	71.96
1.308	3	4 3 4	72.13
1.307	1	7 0 1	72.19
1.302	3	4 6 3	72.56
1.283	3	1 3 5	73.76
1.2739	1	2 8 3	74.41
1.2652	3	6 6 0	75.01
1.2485	1	2 3 5	76.19
1.2438	2	3 0 5	76.53
1.2402	5	7 0 2	76.79
1.2325	1	4 9 0	77.36
1.2291	3	6 3 3	77.62

Potassium zinc iodide hydrate, $\text{KZnI}_3 \cdot 2\text{H}_2\text{O}$

Structure

Orthorhombic, $\text{P2}_1\text{2}_1\text{2}_1$ (19), $Z=4$. The structure was determined by Holinski [private comm., 1973].

Lattice parameters

$a=9.950(3)$, $b=13.727(4)$, $c=7.072(2)\text{\AA}$; published value: $b=13.726$ [ibid]

Density

(calculated) 3.584 g/cm^3

Thermal parameters

Isotropic [Holinski, op. cit.]

Scattering factors

O^0 , K^+ , Zn^{2+} [International Tables, 1962]

I^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 36.27×10^4

Reference

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Holinski, R., Dissertation, 1967; Technischen Hochschule, 3392 Clausthal-Zellerfeld, W. Germany.

International Tables for X-ray Crystallography, III 1962, pgs. 202, 204.

Calculated Pattern (Peak heights)			
$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
8.05	4	1 1 0	10.98
6.86	10	0 2 0	12.90
6.28	6	0 1 1	14.08
5.76	61	1 0 1	15.36
5.65	7	1 2 0	15.68
5.31	8	1 1 1	16.68
4.973	6	2 0 0	17.82
4.924	14	0 2 1	18.00
4.414	2	1 2 1	20.10
4.070	46	2 0 1	21.82
3.900	4	2 1 1	22.78
3.841	18	0 3 1	23.14
3.584	100	1 3 1	24.82
3.537	7	0 0 2	25.16
3.501	3	2 2 1	25.42
3.424	9	0 1 2	26.00
3.368	79	2 3 0	26.44
3.331	88	1 0 2	26.74
3.238	2	1 1 2	27.52
3.225	3	3 1 0	27.64
3.087	2	0 4 1	28.90
3.040	45	2 3 1	29.36
3.004	45	3 0 1 +	29.72
2.934	2	3 1 1	30.44
2.882	1	2 0 2	31.00
2.820	6	2 1 2 +	31.70
2.751	1	3 2 1	32.52
2.693	21	1 3 2	33.24
2.623	2	2 4 1	34.16
2.510	4	3 3 1	35.74
2.439	4	2 3 2	36.82
2.419	1	3 0 2	37.14
2.385	1	3 4 0	37.68
2.347	9	4 0 1	38.32
2.287	25	0 6 0	39.36
2.260	2	3 4 1	39.86
2.220	1	4 2 1	40.60
2.185	18	4 3 0	41.28
2.179	11	1 2 3	41.40
2.139	41	3 3 2	42.22
2.132	27	2 0 3	42.36
2.126	14	1 6 1	42.48
2.105	2	2 1 3	42.92
2.095	8	0 3 3	43.14
2.088	9	4 3 1	43.30
2.051	3	1 3 3	44.12
2.034	2	2 2 3	44.50
2.027	1	3 5 1	44.68
1.994	8	2 6 1	45.44
1.989	6	2 5 2	45.58

Potassium zinc iodide hydrate, $\text{KZnI}_3 \cdot 2\text{H}_2\text{O}$ - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.931	16	2 3 3	47.02
1.921	4	3 0 3 +	47.28
1.916	5	5 0 1	47.42
1.886	19	1 6 2	48.22
1.859	1	4 3 2	48.96
1.857	1	1 7 1	49.02
1.845	1	5 2 1	49.36
1.820	12	3 6 1	50.08
1.815	7	3 5 2	50.22
1.810	2	2 4 3	50.36
1.784	1	4 5 1	51.16
1.767	20	5 3 1 +	51.68
1.741	2	1 0 4	52.52
1.734	2	5 0 2	52.74
1.715	2	0 7 2	53.38
1.711	7	4 0 3	53.52
1.673	1	5 4 1	54.84
1.668	1	0 8 1	55.02
1.658	4	6 0 0	55.36
1.638	4	4 6 1	56.10
1.627	2	1 3 4	56.52
1.622	4	5 3 2 +	56.72
1.602	4	4 3 3	57.46
1.574	1	3 5 3	58.60
1.565	5	2 3 4	58.96
1.559	6	2 6 3	59.22
1.548	1	5 4 2	59.68
1.523	3	6 3 1	60.78
1.476	2	3 3 4	62.90
1.475	3	1 9 1	62.98
1.471	3	3 6 3	63.16
1.469	2	5 6 1	63.26
1.458	2	2 9 0	63.78
1.443	2	5 3 3	64.52
1.428	2	2 9 1	65.28
1.399	4	0 6 4 +	66.82
1.386	1	1 9 2	67.50
1.385	2	1 6 4	67.56
1.382	2	5 6 2	67.74
1.375	4	4 3 4	68.16
1.370	5	4 6 3	68.40
1.3426	3	6 6 0	70.02
1.3393	4	1 3 5	70.22
1.3330	1	7 3 1	70.60
1.3187	3	7 0 2	71.48
1.3005	5	6 3 3 +	72.64
1.2901	3	3 9 2	73.32
1.2805	1	0 9 3	73.96
1.2787	1	4 9 1	74.08
1.2401	2	2 9 3	76.80

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
8.06	3	1 1 0	10.97
6.86	8	0 2 0	12.89
6.29	5	0 1 1	14.08
5.76	52	1 0 1	15.36
5.65	5	1 2 0	15.67
5.31	7	1 1 1	16.67
4.975	5	2 0 0	17.81
4.925	12	0 2 1	18.00
4.414	2	1 2 1	20.10
4.069	45	2 0 1	21.82
3.901	3	2 1 1	22.78
3.842	17	0 3 1	23.13
3.584	100	1 3 1	24.82
3.536	6	0 0 2	25.16
3.500	2	2 2 1	25.43
3.424	7	0 1 2	26.00
3.368	79	2 3 0	26.44
3.332	88	1 0 2	26.73
3.238	2	1 1 2	27.53
3.224	2	3 1 0	27.65
3.087	1	0 4 1	28.89
3.041	49	2 3 1	29.35
3.003	49	3 0 1	29.73
2.997	1	1 2 2	29.78
2.933	1	3 1 1	30.45
2.882	1	2 0 2	31.00
2.825	2	2 4 0	31.65
2.821	5	2 1 2	31.70
2.751	1	3 2 1	32.52
2.693	22	1 3 2	33.24
2.623	2	2 4 1	34.15
2.511	4	3 3 1	35.74
2.439	5	2 3 2	36.83
2.419	1	3 0 2	37.13
2.385	1	3 4 0	37.69
2.347	10	4 0 1	38.33
2.294	2	1 0 3	39.24
2.288	29	0 6 0	39.35
2.276	1	2 5 1	39.57
2.260	1	3 4 1	39.86
2.220	1	4 2 1	40.60
2.185	21	4 3 0	41.28
2.176	1	1 2 3	41.47
2.139	48	3 3 2	42.22
2.130	14	2 0 3	42.40
2.126	7	1 6 1	42.47
2.105	1	2 1 3	42.93
2.096	9	0 3 3	43.13
2.088	8	4 3 1	43.30
2.051	3	1 3 3	44.13

Potassium zinc iodide hydrate, $\text{KZnI}_3 \cdot 2\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.035	2	2 2 3	44.49
2.026	1	3 5 1	44.69
1.994	9	2 6 1	45.44
1.988	3	2 5 2	45.60
1.937	1	4 4 1	46.86
1.931	19	2 3 3	47.01
1.921	2	3 0 3	47.27
1.921	1	0 6 2	47.28
1.916	4	5 0 1	47.42
1.890	1	0 7 1	48.11
1.886	25	1 6 2	48.21
1.859	1	4 3 2	48.96
1.857	1	1 7 1	49.03
1.845	1	5 2 1	49.35
1.820	15	3 6 1	50.08
1.815	1	3 5 2	50.22
1.810	2	2 4 3	50.38
1.784	1	4 5 1	51.17
1.768	9	0 0 4	51.66
1.767	18	5 3 1	51.69
1.741	2	1 0 4	52.53
1.734	2	5 0 2	52.74
1.715	1	0 7 2	53.38
1.711	8	4 0 3	53.51
1.673	1	5 4 1	54.84
1.667	1	0 8 1	55.02
1.658	5	6 0 0	55.35
1.638	4	4 6 1	56.10
1.627	2	1 3 4	56.52
1.622	4	5 3 2	56.72
1.620	1	1 6 3	56.79
1.603	5	4 3 3	57.45
1.574	1	3 5 3	58.59
1.565	7	2 3 4	58.95
1.559	8	2 6 3	59.22
1.548	1	5 4 2	59.69
1.523	3	6 3 1	60.78
1.477	2	3 3 4	62.88
1.474	4	1 9 1	62.99
1.471	1	3 6 3	63.14
1.469	3	5 6 1	63.26
1.458	3	2 9 0	63.77
1.443	2	5 3 3	64.52
1.428	3	2 9 1	65.28
1.400	1	1 0 5	66.74
1.399	6	0 6 4	66.82
1.387	1	1 9 2	67.48
1.385	2	1 6 4	67.56
1.382	2	5 6 2	67.75
1.375	5	4 3 4	68.17

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.370	5	4 6 3	68.41
1.3427	4	6 6 0	70.01
1.3390	4	1 3 5	70.24
1.3331	1	7 3 1	70.59
1.3189	5	7 0 2	71.47
1.3010	3	3 0 5	72.61
1.3004	4	6 3 3	72.65
1.3003	2	4 9 0	72.66
1.2902	5	3 9 2	73.32
1.2806	1	0 9 3	73.96
1.2788	1	4 9 1	74.07
1.2401	2	2 9 3	76.80
1.2095	2	6 0 4	79.11
1.2002	1	8 3 0	79.85
1.1944	1	1 6 5	80.32
1.1932	3	5 9 1	80.41

Sodium D-tartrate hydrate, $(\text{CHOH-CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$

Structure

Orthorhombic, $P2_12_12_1$ (19), $Z=4$. The structure was determined by Ambady and Kartha [1968].

Lattice parameters

$a=11.460(5)$, $b=14.670(5)$, $c=4.959(3)\text{\AA}$ [ibid.]

Density

(calculated) 1.833 g/cm^3

Thermal parameters

Anisotropic [ibid.]

Scattering factors

H^0 , C^0 , O^0 , Na^+ [International Tables, 1962]

Scale factors

(integrated intensities) 2.400×10^4

Reference

Ambady, G.K. and Kartha, G. (1968). Acta Cryst. B24, 1540.

International Tables for X-ray Crystallography III (1962), 202.

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
3.482	22	0 3 1	25.56
3.388	4	3 2 0	26.28
3.331	22	1 3 1 +	26.74
3.089	1	2 4 0	28.88
3.009	2	3 3 0	29.66
2.965	18	3 1 1	30.12
2.864	20	4 0 0	31.20
2.857	25	1 4 1	31.28
2.798	49	3 2 1	31.96
2.668	8	4 2 0	33.56
2.645	4	3 4 0	33.86
2.621	14	2 4 1	34.18
2.614	11	2 5 0	34.28
2.573	8	3 3 1	34.84
2.525	2	0 5 1	35.52
2.481	28	4 0 1 +	36.18
2.473	18	4 3 0	36.30
2.466	12	1 5 1	36.40
2.445	5	4 1 1 +	36.72
2.424	4	1 0 2	37.06
2.391	4	1 6 0	37.58
2.349	5	4 2 1 +	38.28
2.334	1	3 4 1	38.54
2.327	3	3 5 0	38.66
2.311	22	2 5 1	38.94
2.304	13	1 2 2	39.06
2.264	1	5 1 0	39.78
2.258	3	4 4 0	39.90
2.249	6	2 6 0	40.06
2.212	1	0 3 2	40.76
2.187	3	5 2 0	41.24
2.173	5	2 2 2 +	41.52
2.154	9	1 6 1	41.90
2.106	1	3 5 1	42.90
2.080	1	3 0 2	43.48
2.062	10	2 3 2 +	43.88
2.054	11	4 4 1 +	44.04
2.050	6	4 5 0	44.14
2.022	1	1 4 2	44.78
2.001	4	5 2 1 +	45.28
1.968	2	2 7 0	46.08
1.933	2	2 4 2	46.96
1.930	2	0 7 1	47.04
1.914	4	3 3 2	47.46
1.904	3	1 7 1	47.74
1.894	4	6 1 0 +	48.00
1.860	8	4 1 2 +	48.94

Calculated Pattern (*Peak heights*)

$d\text{ (\AA)}$	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056\text{ \AA}$
9.02	100	1 1 0	9.80
6.171	10	1 2 0	14.34
5.727	29	2 0 0	15.46
4.696	25	0 1 1	18.88
4.548	14	1 0 1	19.50
4.498	22	1 3 0	19.72
3.867	6	1 2 1	22.98
3.720	2	2 3 0	23.90
3.666	4	0 4 0	24.26
3.633	35	2 1 1	24.48

Sodium D-tartrate hydrate, $(\text{CHOH-CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$ - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.848	3	6 2 0	49.26
1.837	1	3 7 0	49.58
1.829	3	2 7 1	49.80
1.817	4	4 2 2	50.18
1.810	3	5 4 1	50.38
1.806	2	5 5 0	50.50
1.798	7	2 5 2	50.72
1.779	2	6 3 0	51.32
1.769	1	6 1 1	51.62
1.750	1	4 3 2	52.22
1.747	2	2 8 0	52.34
1.742	2	4 6 1	52.50
1.732	1	6 2 1	52.82
1.721	2	1 6 2	53.16
1.701	1	1 8 1	53.86
1.697	3	5 5 1 +	54.00
1.694	4	6 4 0	54.10
1.647	2	2 8 1	55.76
1.636	1	1 0 3	56.16
1.626	1	1 1 3	56.56
1.600	1	6 5 0 +	57.54
1.597	3	1 2 3 +	57.68
1.592	2	5 3 2	57.88
1.584	3	5 6 1 +	58.18
1.580	2	2 1 3	58.36
1.568	2	3 8 1	58.84
1.555	2	7 0 1	59.40
1.551	3	1 3 3	59.54
1.547	2	7 1 1 +	59.72
1.542	1	2 7 2	59.94
1.517	1	3 0 3	61.02
1.513	1	6 0 2	61.20
1.511	3	2 3 3 +	61.32
1.505	2	6 1 2	61.56
1.495	1	7 4 0	62.04
1.488	1	4 6 2	62.36
1.486	1	3 2 3	62.46
1.482	2	7 3 1 +	62.64
1.477	1	5 7 1	62.88
1.467	1	0 10 0	63.34
1.432	1	7 4 1 +	65.10
1.428	2	2 8 2 +	65.28
1.417	1	4 9 0	65.86
1.412	1	6 7 0	66.14
1.370	1	8 1 1	68.42
1.227	1	6 7 2	77.78
1.222	1	0 2 4	78.12
1.220	1	5 5 3	78.34
1.175	1	0 11 2	81.96

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
9.03	100	1 1 0	9.79
6.178	11	1 2 0	14.32
5.730	32	2 0 0	15.45
4.698	28	0 1 1	18.67
4.551	15	1 0 1	19.49
4.516	4	2 2 0	19.64
4.498	24	1 3 0	19.72
3.867	7	1 2 1	22.98
3.720	2	2 3 0	23.90
3.667	4	0 4 0	24.25
3.633	44	2 1 1	24.48
3.482	27	0 3 1	25.56
3.388	5	3 2 0	26.28
3.339	13	2 2 1	26.66
3.332	19	1 3 1	26.74
3.089	1	2 4 0	28.88
3.010	2	3 3 0	29.65
2.964	25	3 1 1	30.13
2.865	24	4 0 0	31.19
2.856	24	1 4 1	31.30
2.797	68	3 2 1	31.97
2.669	11	4 2 0	33.55
2.646	5	3 4 0	33.85
2.622	20	2 4 1	34.17
2.612	8	2 5 0	34.31
2.573	11	3 3 1	34.84
2.525	2	0 5 1	35.52
2.481	36	4 0 1	36.18
2.479	3	0 0 2	36.20
2.472	5	4 3 0	36.31
2.466	11	1 5 1	36.40
2.446	4	4 1 1	36.71
2.445	2	0 6 0	36.73
2.423	5	1 0 2	37.07
2.391	6	1 6 0	37.58
2.350	7	4 2 1	38.27
2.349	1	0 2 2	38.29
2.334	1	3 4 1	38.54
2.327	3	3 5 0	38.66
2.311	32	2 5 1	38.94
2.301	2	1 2 2	39.11
2.265	1	5 1 0	39.77
2.258	4	4 4 0	39.90
2.249	7	2 6 0	40.06
2.211	1	0 3 2	40.77
2.193	1	0 6 1	41.13
2.188	4	5 2 0	41.23
2.173	6	2 2 2	41.51
2.171	3	1 3 2	41.55
2.154	13	1 6 1	41.91

Sodium D-tartrate hydrate, $(\text{CHOH-CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$ – continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.106	1	3 5 1	42.90
2.080	1	3 0 2	43.48
2.063	8	2 3 2	43.85
2.062	7	1 7 0	43.88
2.060	2	5 1 1	43.92
2.059	2	3 1 2	43.93
2.055	8	4 4 1	44.03
2.054	3	0 4 2	44.05
2.050	2	4 5 0	44.14
2.022	2	1 4 2	44.79
2.002	3	5 2 1	45.27
2.001	3	3 2 2	45.28
1.968	3	2 7 0	46.08
1.934	3	2 4 2	46.95
1.930	2	0 7 1	47.03
1.914	6	3 3 2	47.47
1.904	4	1 7 1	47.74
1.894	5	6 1 0	47.99
1.894	1	0 5 2	48.00
1.860	2	4 6 0	48.93
1.860	11	4 1 2	48.94
1.848	4	6 2 0	49.26
1.837	1	3 7 0	49.57
1.829	4	2 7 1	49.80
1.816	7	4 2 2	50.18
1.810	3	5 4 1	50.38
1.806	1	5 5 0	50.49
1.798	12	2 5 2	50.73
1.779	3	6 3 0	51.31
1.769	2	6 1 1	51.61
1.751	1	4 3 2	52.21
1.746	3	2 8 0	52.34
1.741	2	4 6 1	52.51
1.732	1	6 2 1	52.81
1.721	3	1 6 2	53.17
1.701	1	1 8 1	53.86
1.697	2	5 5 1	53.98
1.697	2	3 5 2	54.00
1.694	5	6 4 0	54.09
1.675	1	6 3 1	54.77
1.647	4	2 8 1	55.76
1.636	1	1 0 3	56.17
1.626	2	1 1 3	56.55
1.601	1	4 7 1	57.52
1.601	1	6 5 0	57.53
1.598	2	7 2 0	57.64
1.597	3	1 2 3	57.68
1.591	2	5 3 2	57.90
1.585	2	5 6 1	58.17
1.584	2	3 6 2	58.19

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.579	1	2 1 3	58.40
1.568	2	3 8 1	58.83
1.555	3	7 0 1	59.40
1.552	4	1 3 3	59.53
1.548	1	0 9 1	59.66
1.547	1	5 7 0	59.74
1.546	1	7 1 1	59.77
1.542	1	2 7 2	59.96
1.523	1	6 5 1	60.75
1.517	1	3 0 3	61.03
1.513	1	6 0 2	61.20
1.511	4	2 3 3	61.32
1.509	1	3 1 3	61.39
1.505	1	6 1 2	61.56
1.495	2	7 4 0	62.03
1.488	2	4 6 2	62.36
1.486	1	3 2 3	62.46
1.482	1	6 2 2	62.64
1.482	1	7 3 1	62.65
1.476	1	5 7 1	62.89
1.467	2	0 10 0	63.35
1.460	1	5 5 2	63.69
1.432	1	5 8 0	65.09
1.431	1	7 4 1	65.12
1.430	1	7 5 0	65.20
1.429	1	1 5 3	65.24
1.428	1	2 8 2	65.30
1.417	1	4 9 0	65.87
1.412	1	6 7 0	66.14
1.370	1	8 1 1	68.41
1.362	1	0 9 2	68.88
1.353	1	8 2 1	69.43
1.348	1	3 5 3	69.72
1.227	1	6 7 2	77.79
1.222	1	0 2 4	78.12
1.219	1	5 5 3	78.35
1.175	1	0 11 2	81.96

Yttrium titanium oxide, Y₂TiO₅

Structure

Orthorhombic, Pnam (62), Z=4. The structure was determined by Mumme and Wadsley (1968).

Lattice parameters

a=10.35(1), b=11.25(1), c=3.70(1) Å [ibid.]

Density

(calculated) 4.713 g/cm³

Thermal parameters

Isotropic [ibid.]

Scattering factors

O²⁻ [Suzuki, 1960]

Y³⁺, Ti⁴⁺ [Cromer and Waber, 1965]. These factors were corrected for dispersion [Cromer, 1965].

Scale factors

(integrated intensities) 10.05 × 10⁴

Additional patterns

1. PDF card 21-1464 [Garton and Wanklyn, 1968]

Reference

Cromer, D.T. (1965). Acta Cryst. 18, 17.

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Garton, G. and Wanklyn, B.M. (1968). J. Mater.Sci. 3, 395.

Mumme, W.G. and Wadsley, A.D. (1968). Acta Cryst. B24, 1327.

Suzuki, T. (1960). Acta Cryst. 13, 279.

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
2.94	9	3 2 0	30.36
2.91	4	2 1 1	30.72
2.71	2	1 4 0	32.98
2.63	25	0 3 1	34.02
2.587	8	4 0 0	34.64
2.552	9	1 3 1	35.14
2.539	8	3 3 0	35.32
2.521	4	4 1 0	35.58
2.462	3	3 1 1	36.46
2.302	7	3 2 1	39.10
2.198	4	1 5 0	41.02
2.130	1	4 3 0	42.40
2.121	2	4 0 1	42.60
2.093	8	3 3 1	43.18
2.084	4	4 1 1	43.38
2.055	3	2 4 1	44.02
2.036	2	5 1 0	44.46
1.984	3	4 2 1	45.68
1.943	1	5 2 0	46.72
1.904	3	4 4 0	47.72
1.890	1	1 5 1	48.10
1.875	4	0 6 0	48.52
1.850	23	0 0 2	49.22
1.845	55	4 3 1 +	49.34
1.798	1	1 1 2	50.74
1.783	2	5 1 1	51.18
1.720	6	5 2 1	53.20
1.705	1	6 1 0	53.72
1.693	1	4 4 1	54.12
1.679	2	3 5 1	54.60
1.667	1	5 4 0	55.04
1.651	10	1 6 1 +	55.62
1.647	7	3 6 0	55.76
1.638	4	1 3 2	56.10
1.627	4	5 3 1	56.50
1.591	5	2 6 1	57.90
1.580	15	2 3 2	58.36
1.567	5	6 3 0 +	58.88
1.563	7	6 0 1	59.04
1.549	2	6 1 1	59.66
1.524	1	5 5 0	60.74
1.519	2	4 6 0	60.96
1.505	10	3 6 1 +	61.58
1.495	2	3 3 2	62.02
1.492	2	4 1 2	62.18
1.470	1	6 4 0	63.18
1.466	2	7 1 0	63.38
1.443	1	6 3 1	64.52
1.430	1	7 2 0	65.18
1.418	1	2 7 1	65.82
1.415	1	1 5 2	65.94

Calculated Pattern (Peak heights)

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
7.61	18	1 1 0	11.62
5.63	2	0 2 0	15.74
5.18	11	2 0 0	17.12
4.94	3	1 2 0	17.94
4.70	6	2 1 0	18.86
3.81	2	2 2 0	23.34
3.53	24	1 3 0 +	25.24
3.33	2	1 1 1	26.76
3.04	74	2 3 0	29.40
3.01	100	2 0 1	29.66

Yttrium titanium oxide, Y_2TiO_5 - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.390	2	5 6 0	67.32
1.369	1	5 1 2	68.48
1.367	2	6 4 1	68.62
1.363	1	7 1 1	68.82
1.327	1	4 4 2	70.98
1.317	1	0 6 2	71.60
1.306	6	1 6 2	72.26
1.294	1	8 0 0	73.08
1.285	1	8 1 0	73.64
1.281	1	4 7 1	73.94
1.241	1	1 9 0	76.74
1.234	1	7 4 1	77.26
1.230	1	3 6 2 +	77.52
1.200	4	2 0 3 +	79.88
1.196	3	6 3 2	80.20
1.193	2	8 2 1	80.44
1.176	4	1 9 1 +	81.88
1.174	4	4 6 2	82.04
1.172	4	0 3 3 +	82.20
1.164	1	1 3 3	82.86
1.161	1	8 3 1	83.12
1.151	1	6 4 2	84.00
1.149	1	7 1 2	84.20
1.131	1	7 2 2	85.82
1.120	2	3 9 1	86.90
1.111	2	5 6 2	87.78
1.109	2	5 8 1 +	87.94
1.108	2	7 6 1	88.10
1.104	1	7 3 2	88.50
1.093	1	9 1 1	89.62
1.070	1	5 9 0	92.08
1.067	3	4 3 3	92.40
1.060	1	8 0 2	93.20
1.055	1	8 1 2	93.74
1.044	1	7 7 1	95.10
1.041	1	5 2 3	95.42
1.031	2	1 9 2	96.74
1.028	3	5 9 1	97.08
1.025	3	1 6 3	97.40
1.020	1	5 3 3	98.14
1.011	1	2 6 3	99.32
1.003	1	6 0 3	100.30
.992	3	3 9 2 +	101.88
.987	2	3 6 3	102.56
.972	1	8 7 1	104.78
.939	1	10 4 1	110.16
.934	1	1 12 0	111.18
.926	1	5 9 2	112.54
.925	1	0 0 4	112.76
.923	2	8 6 2 +	113.20
.911	1	10 5 1	115.40

Calculated Pattern (Integrated)			
d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
7.62	14	1 1 0	11.61
5.63	2	0 2 0	15.74
5.18	10	2 0 0	17.12
4.94	2	1 2 0	17.93
4.70	5	2 1 0	18.86
3.81	2	2 2 0	23.34
3.53	24	1 3 0	25.24
3.51	1	0 1 1	25.32
3.33	2	1 1 1	26.76
3.04	78	2 3 0	29.39
3.01	100	2 0 1	29.66
2.94	9	3 2 0	30.37
2.91	4	2 1 1	30.72
2.71	2	1 4 0	32.98
2.63	27	0 3 1	34.01
2.588	8	4 0 0	34.64
2.552	10	1 3 1	35.13
2.539	8	3 3 0	35.32
2.522	4	4 1 0	35.57
2.462	3	3 1 1	36.46
2.302	8	3 2 1	39.09
2.199	4	1 5 0	41.02
2.188	1	1 4 1	41.22
2.130	1	4 3 0	42.41
2.120	2	4 0 1	42.60
2.093	9	3 3 1	43.18
2.084	4	4 1 1	43.39
2.055	3	2 4 1	44.03
2.036	2	5 1 0	44.46
1.984	4	4 2 1	45.69
1.943	1	5 2 0	46.72
1.904	3	4 4 0	47.72
1.890	1	1 5 1	48.10
1.878	2	3 4 1	48.42
1.875	4	0 6 0	48.51
1.850	22	0 0 2	49.21
1.846	43	4 3 1	49.33
1.845	16	1 6 0	49.35
1.798	1	1 1 2	50.74
1.784	2	5 1 1	51.17
1.720	7	5 2 1	53.21
1.705	2	6 1 0	53.71
1.693	2	4 4 1	54.12
1.679	3	3 5 1	54.60
1.667	1	5 4 0	55.04
1.651	13	1 6 1	55.62
1.649	1	6 2 0	55.69
1.647	1	3 6 0	55.75
1.638	4	1 3 2	56.10
1.627	5	5 3 1	56.50

Yttrium titanium oxide, Y_2TiO_5 - continued

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.591	6	2 6 1	57.90
1.580	20	2 3 2	58.36
1.567	5	6 3 0	58.88
1.566	2	3 2 2	58.93
1.563	7	6 0 1	59.03
1.549	3	6 1 1	59.66
1.523	2	5 5 0	60.75
1.518	2	4 6 0	60.97
1.505	9	3 6 1	61.57
1.505	4	4 0 2	61.57
1.495	3	3 3 2	62.02
1.492	1	4 1 2	62.18
1.474	1	0 7 1	63.01
1.470	2	6 4 0	63.18
1.466	2	7 1 0	63.40
1.443	1	6 3 1	64.52
1.430	2	7 2 0	65.18
1.418	1	2 7 1	65.82
1.416	2	1 5 2	65.93
1.390	2	5 6 0	67.32
1.376	1	7 3 0	68.11
1.369	1	5 1 2	68.47
1.367	2	6 4 1	68.62
1.363	1	7 1 1	68.83
1.327	2	4 4 2	70.97
1.317	2	0 6 2	71.59
1.306	9	1 6 2	72.26
1.301	1	5 6 1	72.61
1.294	2	8 0 0	73.08
1.285	1	8 1 0	73.64
1.281	1	4 7 1	73.94
1.254	1	6 1 2	75.81
1.241	2	1 9 0	76.73
1.234	1	7 4 1	77.26
1.231	1	6 2 2	77.47
1.230	1	3 6 2	77.52
1.214	1	8 1 1	78.76
1.201	2	6 6 1	79.81
1.200	5	2 0 3	79.89
1.196	4	6 3 2	80.21
1.193	1	8 2 1	80.40
1.177	4	1 9 1	81.79
1.176	1	5 5 2	81.84
1.176	1	6 7 0	81.85
1.175	1	8 4 0	81.89
1.175	3	3 9 0	81.90
1.174	2	4 6 2	82.04
1.172	2	7 5 1	82.18
1.172	3	0 3 3	82.21
1.164	1	1 3 3	82.85

d (Å)	I	hkl	$2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$
1.161	2	8 3 1	83.11
1.151	1	6 4 2	84.00
1.149	1	7 1 2	84.20
1.131	1	7 2 2	85.82
1.120	3	3 9 1	86.90
1.111	2	5 6 2	87.78
1.110	1	5 8 1	87.92
1.109	1	3 3 3	87.95
1.108	2	7 6 1	88.11
1.104	1	7 3 2	88.51
1.093	1	9 1 1	89.62
1.078	1	9 2 1	91.23
1.070	1	5 9 0	92.09
1.067	6	4 3 3	92.39
1.060	2	8 0 2	93.19
1.056	1	8 1 2	93.73
1.044	1	7 7 1	95.10
1.041	1	5 2 3	95.43
1.031	2	1 9 2	96.73
1.028	4	5 9 1	97.07
1.025	3	1 6 3	97.40
1.024	1	9 5 0	97.57
1.020	1	5 3 3	98.13
1.011	1	2 6 3	99.32
1.003	2	6 0 3	100.31
.993	1	10 1 1	101.76
.992	1	6 7 2	101.83
.992	1	8 4 2	101.87
.992	4	3 9 2	101.88
.987	3	3 6 3	102.55
.972	2	8 7 1	104.78
.962	1	9 2 2	106.35
.959	1	8 5 2	106.86
.955	1	5 10 1	107.53
.955	1	7 9 0	107.59
.945	1	6 4 3	109.20
.939	2	10 4 1	110.15
.934	1	1 12 0	111.18
.926	1	5 9 2	112.53
.925	2	0 0 4	112.76
.923	1	8 6 2	113.16
.923	1	9 4 2	113.21
.911	2	10 5 1	115.39

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Ammonium copper chloride, NH ₄ CuCl ₄	7m	7	Antimony(IV) oxide (cervantite), Sb ₂ O ₄	10	8
Ammonium copper chloride hydrate, (NH ₄) ₂ CuCl ₄ ·2H ₂ O	9m	8	Antimony(V) oxide, Sb ₂ O ₅	10	10
Ammonium copper fluoride, NH ₄ CuF ₃	11m	8	Antimony, Sb	3	14
Ammonium gallium sulfate hydrate, NH ₄ Ga(SO ₄) ₂ ·12H ₂ O	6	9	Antimony selenide, Sb ₂ Se ₃	3m	7
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Ammonium hydrogen carbonate (teschemache- rite), (NH ₄)HCO ₃	9	5	Antimony telluride, Sb ₂ Te ₃	3m	8
Ammonium hydrogen phosphate, NH ₄ H ₂ PO ₄ ..	4	64	Arsenic, As	3	6
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⁵ Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

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Barium bromide hydrate, BaBr ₂ ·H ₂ O	3m	10	Cadmium bromide, CdBr ₂	9	17
Barium calcium tungsten oxide, Ba ₂ CaWO ₆ ...	9m	10	Cadmium bromide chloride, CdBrCl	11m	15
Barium carbonate (witherite), BaCO ₃ (ortho- rhombic)	2	54	Cadmium carbonate (otavite), CdCO ₃	7	11
Barium carbonate, BaCO ₃ (cubic) at 1075 °C ..	10	11	Cadmium chlorate hydrate, Cd(ClO ₄) ₂ ·2H ₂ O ...	3m	19
Barium chlorate hydrate, Ba(ClO ₄) ₂ ·3H ₂ O	2m	7	Cadmium chloride, CdCl ₂	9	18
Barium chlorate hydrate, Ba(ClO ₃) ₂ ·H ₂ O	8m	21	Cadmium chromium oxide, CdCr ₂ O ₄	5m	16
Barium chloride, BaCl ₂ , (orthorhombic)	9m	11	Cadmium cyanide, Cd(CN) ₂	2m	8
Barium chloride, BaCl ₂ , (cubic)	9m	13	Cadmium fluoride, CdF ₂	10m	15
Barium chloride fluoride, BaClF	10m	11	Cadmium iron oxide, CdFe ₂ O ₄	9m	16
Barium fluoride, BaF ₂	1	70	Cadmium manganese oxide, CdMn ₂ O ₄	10m	16
Barium hydroxide phosphate, Ba ₅ (OH)(PO ₄) ₃	11m	12	Cadmium molybdenum oxide, CdMoO ₄	6	21
Barium iodide, BaI ₂	10m	66	Cadmium nitrate hydrate, Cd(NO ₃) ₂ ·4H ₂ O	7m	93
Barium lead chloride, BaPbCl ₄	11m	13	Cadmium oxide, CdO	2	27
Barium molybdenum oxide, BaMoO ₄	7	7	Cadmium oxide, CdO (ref. standard)	8m	2
Barium nitrate (nitrobarite), Ba(NO ₃) ₂ (revised)	11m	14	Cadmium selenide, CdSe (hexagonal)	7	12
Barium oxide, BaO	9m	63	Cadmium sulfate, CdSO ₄	3m	20
Barium oxide, BaO ₂	6	18	Cadmium sulfate hydrate, 3CdSO ₄ ·8H ₂ O	6m	8
Barium selenide, BaSe	5m	61	Cadmium sulfate hydrate, CdSO ₄ ·H ₂ O	6m	10
Barium silicon fluoride, BaSiF ₆	4m	7	Cadmium sulfide (greenockite), CdS	4	15
Barium sulfate (barite), BaSO ₄ (revised)	10m	12	Cadmium telluride, CdTe	3m	21
Barium sulfide, BaS	7	8	Cadmium tungsten oxide, CdWO ₄	2m	8
Barium tin oxide, BaSnO ₃	3m	11	Calcium, Ca	9m	68
Barium titanium oxide, BaTiO ₃	3	45	Calcium aluminum germanium oxide, Ca ₃ Al ₂ (GeO ₄) ₃	10	15
Barium titanium silicate (fresnoite), Ba ₂ TiSi ₂ O ₈	9m	14	Calcium aluminum hydroxide, Ca ₃ Al ₂ (OH) ₁₂ ..	11m	16
Barium tungsten oxide, BaWO ₄	7	9	Calcium aluminum oxide, Ca ₃ Al ₂ O ₆	5	10
Barium zirconium oxide, BaZrO ₃	5	8	Calcium aluminum oxide, 12CaO·7Al ₂ O ₃	9	20
Beryllium, alpha, Be	9m	64	Calcium aluminum sulfate hydrate (ettringite), 6CaO·Al ₂ O ₃ ·3SO ₃ ·31H ₂ O	8	3
Beryllium aluminum oxide (chrysoberyl), BeAl ₂ O ₄	9	10	Calcium Bromide, CaBr ₂	11m	70
Beryllium aluminum silicate, beryl, Be ₃ Al ₂ (SiO ₃) ₆	9	13	Calcium bromide hydrate, CaBr ₂ ·6H ₂ O	8	15
Beryllium calcium oxide, Be ₇ Ca ₁₀ O ₁₈	7m	89	Calcium carbonate (aragonite), CaCO ₃ (orthorhombic)	3	53
Beryllium chromium oxide, BeCr ₂ O ₄	10	12	Calcium carbonate (calcite) CaCO ₃ (hexagonal)	2	51
Beryllium cobalt, BeCo	5m	62	Calcium chloride fluoride, CaClF	10m	17
Beryllium germanium oxide, Be ₂ GeO ₄	10	13	Calcium chloride (hydrophilite), CaCl ₂	11m	18
Beryllium lanthanum oxide, Be ₂ La ₂ O ₅	9m	65	Calcium chloride hydrate, CaCl ₂ ·4H ₂ O	11m	73
Beryllium niobium, Be ₂ Nb	7m	92	Calcium chromium germanium oxide, Ca ₃ Cr ₂ (GeO ₄) ₃	10	16
Beryllium oxide (bromellite), BeO	1	36	Calcium chromium oxide, CaCrO ₄	7	13
Beryllium palladium, BePd	5m	62	Calcium chromium silicate (uvavovite), Ca ₃ Cr ₂ (SiO ₄) ₃	10	17
Beryllium silicate, phenacite, BeSi ₂ O ₄	8	11	Calcium fluoride (fluorite), CaF ₂	1	69
Bismuth, Bi	3	20	Calcium fluoride phosphate (fluorapatite), Ca ₅ F(PO ₄) ₃	3m	22
Bismuth fluoride, BiF ₃	1m	7	Calcium gallium germanium oxide, Ca ₃ Ga ₂ (GeO ₄) ₃	10	18
Bismuth(III) iodide, BiI ₃	6	20	Calcium hydroxide (portlandite), Ca(OH) ₂	1	58
Bismuth oxide (bismite), alpha Bi ₂ O ₃	3m	16	Calcium iron germanium oxide, Ca ₃ Fe ₂ (GeO ₄) ₃	10	19
Bismuth oxide bromide, BiOBr	8	14	Calcium iron silicate (andradite), Ca ₃ Fe ₂ Si ₃ O ₁₂	9	22
Bismuth oxide chloride (bismoclite), BiOCl ..	4	54	Calcium iron silicate hydroxide, julgoldite, Ca ₂ Fe ₃ Si ₃ O ₁₀ (OH, O) ₂ (OH) ₂	10m	72
Bismuth oxide iodide, BiOI	9	16	Calcium magnesium silicate (diopside), CaMg(SiO ₃) ₂	5m	17
Bismuth phosphate, BiPO ₄ (monoclinic)	3m	11	Calcium molybdenum oxide (powellite), CaMoO ₄	6	22
Bismuth phosphate, BiPO ₄ (trigonal)	3m	13	Calcium nitrate, Ca(NO ₃) ₂	7	14
Bismuth sulfide (bismuthinite), Bi ₂ S ₃ (revised)	5m	13	Calcium oxide, CaO	1	43
Bismuth telluride, BiTe	4m	50	Calcium phosphate, beta Ca ₃ P ₂ O ₇	7m	95
Bismuth telluride (tellurobismuthite), Bi ₂ Te ₃	3m	16	Calcium platinum oxide, Ca ₄ PtO ₆	10m	18
Bismuth vanadium oxide, low form, BiVO ₄ (tetragonal)	3m	14	Calcium selenide, CaSe	5m	64
Bismuth vanadium oxide, high form, BiVO ₄ (monoclinic)	3m	14	Calcium sulfate (anhydrite), CaSO ₄	4	65
Boric acid, HBO ₂ (cubic)	4m	27	Calcium sulfide (oldhamite), CaS	7	15
Boron oxide, B ₂ O ₃ , phase 1	10m	70	Calcium telluride, CaTe	4m	50
Cadmium, Cd	3	10			
Cadmium ammine chloride, Cd(NH ₃) ₂ Cl ₂	10m	14			

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Calcium titanium oxide (perovskite), CaTiO ₃	9m	17	Cesium lithium fluoride, CsLiF ₃	7m	105
Calcium tungsten oxide, Ca ₃ WO ₆	9m	19	Cesium magnesium chromium oxide, Cs ₂ Mg ₂ (CrO ₄) ₃	8m	27
Calcium tungsten oxide, scheelite, CaWO ₄	6	23	Cesium magnesium chromium oxide hydrate, Cs ₂ Mg(CrO ₄) ₂ ·6H ₂ O	8m	29
Carbon, diamond, C	2	5	Cesium manganese fluoride, CsMnF ₃	10m	21
Cerium antimony, CeSb	4m	40	Cesium magnesium sulfate hydrate, Cs ₂ Mg(SO ₄) ₂ ·6H ₂ O	7m	18
Cerium arsenate, CeAsO ₄	4m	8	Cesium manganese sulfate hydrate, Cs ₂ Mn(SO ₄) ₂ ·6H ₂ O	7m	20
Cerium arsenide, CeAs	4m	51	Cesium mercury chloride, CsHgCl ₃	7m	22
Cerium bismuth, CeBi	4m	46	Cesium nickel(II) chloride, CsNiCl ₃	6m	12
Cerium cadmium, CeCd	5m	63	Cesium nickel sulfate hydrate, Cs ₂ Ni(SO ₄) ₂ ·6H ₂ O	7m	23
Cerium(III) chloride, CeCl ₃	1m	8	Cesium nitrate, CsNO ₃	9	25
Cerium copper, CeCu	7m	99	Cesium osmium(IV) bromide, Cs ₂ OsBr ₆	2m	10
Cerium(III) fluoride, CeF ₃	8	17	Cesium osmium chloride, Cs ₂ OsCl ₆	2m	11
Cerium niobium titanium oxide (eschynite), CeNbTiO ₆	3m	24	Cesium platinum bromide, Cs ₂ PtBr ₆	8	19
Cerium nitride, CeN	4m	51	Cesium platinum chloride, Cs ₂ PtCl ₆	5	14
Cerium(IV) oxide (cerianite), CeO ₂	1	56	Cesium platinum fluoride, Cs ₂ PtF ₆	6	27
Cerium phosphide, CeP	4m	52	Cesium selenium bromide, Cs ₂ SeBr ₆	8	20
Cerium(III) vanadium oxide, CeVO ₄	1m	9	Cesium silicon fluoride, Cs ₂ SiF ₆	5	19
Cerium zinc, CeZn	5m	65	Cesium strontium chloride, CsSrCl ₃	6m	13
Cesium aluminum sulfate hydrate, CsAl(SO ₄) ₂ ·12H ₂ O	6	25	Cesium sulfate Cs ₂ SO ₄	7	17
Cesium antimony fluoride, CsSbF ₆	4m	9	Cesium tellurium bromide, Cs ₂ TeBr ₆	9	24
Cesium beryllium fluoride, CsBeF ₃	9m	69	Cesium tin chloride, Cs ₂ SnCl ₆	5	16
Cesium boron fluoride, CsBF ₄	8	22	Cesium vanadium sulfate hydrate, CsV(SO ₄) ₂ ·12H ₂ O	1m	11
Cesium bromate, CsBrO ₃	8	18	Cesium zinc sulfate hydrate, Cs ₂ Zn(SO ₄) ₂ ·6H ₂ O	7m	25
Cesium bromide, CsBr	3	49	Chromium, Cr	5	20
Cesium cadmium bromide, CsCdBr ₃ (hexagonal)	10m	20	Chromium chloride, CrCl ₂	11m	77
Cesium cadmium chloride, CsCdCl ₃ (hexagonal)	5m	19	Chromium fluoride, CrF ₃	7m	108
Cesium calcium chloride, CsCaCl ₃	5m	21	Chromium fluoride, CrF ₂	10m	81
Cesium calcium fluoride, CsCaF ₃	8m	25	Chromium(III) fluoride hydrate, CrF ₃ ·3H ₂ O	5m	25
Cesium calcium sulfate, Cs ₂ Ca ₂ (SO ₄) ₄	7m	12	Chromium iridium 3:1, Cr ₃ Ir	6m	14
Cesium cerium chloride, Cs ₂ CeCl ₆	7m	101	Chromium(III) oxide, Cr ₂ O ₃	5	22
Cesium chlorate, CsClO ₃	8	20	Chromium phosphate, alpha CrPO ₄	2m	12
Cesium chlorate, CsClO ₄ (orthorhombic)	1m	10	Chromium phosphate, beta CrPO ₄	9	26
Cesium chloride, CsCl	2	44	Chromium rhodium 3:1, Cr ₃ Rh	6m	15
Cesium chromium oxide, Cs ₂ CrO ₄	3m	25	Chromium silicide, Cr ₃ Si	6	29
Cesium chromium sulfate hydrate, CsCr(SO ₄) ₂ ·12H ₂ O	8	21	Cobalt, Co (cubic)	4m	10
Cesium cobalt(II) chloride, CsCoCl ₃	6m	11	Cobalt aluminum oxide, CoAl ₂ O ₄	9	27
Cesium cobalt chloride, Cs ₂ CoCl ₄	11m	19	Cobalt ammine iodide, Co(NH ₃) ₅ I ₃	10m	83
Cesium copper(II) chloride, CsCuCl ₃	5m	22	Cobalt antimony oxide, CoSb ₂ O ₆	5m	26
Cesium copper chloride, Cs ₂ CuCl ₄	11m	20	Cobalt arsenide, CoAs ₂ (revised)	4m	10
Cesium copper sulfate hydrate, Cs ₂ Cu(SO ₄) ₂ ·6H ₂ O	7m	14	Cobalt arsenide (skutterudite), CoAs ₃	10	21
Cesium fluoride, CsF	3m	26	Cobalt(II) carbonate (spherocobaltite), CoCO ₃	10	24
Cesium gallium sulfate hydrate, CsGa(SO ₄) ₂ ·12H ₂ O	8	23	Cobalt chlorate hydrate, Co(ClO ₄) ₂ ·6H ₂ O	3m	28
Cesium germanium fluoride, Cs ₂ GeF ₆	5	17	Cobalt chloride hydrate, CoCl ₂ ·2H ₂ O	11m	22
Cesium iodide, CsI	4	47	Cobalt chloride hydrate, CoCl ₂ ·6H ₂ O	11m	23
Cesium iodine bromide, CsI ₂ Br	7m	103	Cobalt chromium oxide, CoCr ₂ O ₄	9m	21
Cesium iodine chloride, CsICl ₂	3	50	Cobalt fluoride, CoF ₂	10m	85
Cesium iron sulfate hydrate, Cs ₂ Fe(SO ₄) ₂ ·6H ₂ O	7m	16	Cobalt fluoride hydrate, CoF ₂ ·4H ₂ O	11m	24
Cesium iron sulfate hydrate, CsFe(SO ₄) ₂ ·12H ₂ O	6	28	Cobalt gallium oxide, CoGa ₂ O ₄	10	27
Cesium lead(II) chloride, CsPbCl ₃ (tetragonal)	5m	24	Cobalt germanium oxide, Co ₂ GeO ₄	10	27
Cesium lead fluoride, CsPbF ₃	8m	26	Cobalt iodide, CoI ₂	4m	52
Cesium lithium cobalt cyanide, CsLiCo(CN) ₆	10m	79	Cobalt iron arsenide (safflorite), CoFeAs ₄	10	28
			Cobalt iron oxide, CoFe ₂ O ₄	9m	22
			Cobalt mercury thiocyanate, Co[Hg(CNS) ₂]	2m	13
			Cobalt(II) oxide, CoO	9	28
			Cobalt(II, III) oxide, Co ₃ O ₄	9	29
			Cobalt silicate, Co ₂ SiO ₄ (orthorhombic)	4m	11
			Cobalt silicon fluoride hydrate, CoSiF ₆ ·6H ₂ O	3m	27

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Cobalt sulfate, beta, CoSO_4	2m	14	Gadolinium gallium oxide, $\text{Gd}_3\text{Ga}_2(\text{GaO}_4)_3$	2m	18
Cobalt titanium oxide, CoTiO_3	4m	13	Gadolinium indium, GdIn	5m	67
Cobalt tungsten oxide, CoWo_4	4m	13	Gadolinium nitride, GdN	4m	57
Copper, Cu	1	15	Gadolinium oxide, Gd_2O_3	1m	16
Copper aluminum, Cu_3Al_4	11m	79	Gadolinium oxychloride, GdOCl	1m	17
Copper ammine selenate, $\text{Cu}(\text{NH}_3)_4\text{SeO}_4$	10m	87	Gadolinium silver, GdAg	6m	87
Copper ammine sulfate hydrate, $\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$	10m	90	Gadolinium titanium oxide, Gd_2TiO_5	8m	32
Copper antimony oxide, CuSb_2O_6	5m	27	Gadolinium vanadium oxide, GdVO_4	5m	30
Copper(I) bromide, CuBr	4	36	Gallium, Ga	2	9
Copper cadmium, Cu_5Cd_8	11m	81	Gallium antimony, GaSb	6	30
Copper(I) chloride (nantokite), CuCl	4	35	Gallium arsenide, GaAs	3m	33
Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$	11m	25	Gallium oxide, alpha, Ga_2O_3	4	25
Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$	11m	83	Gallium phosphate hydrate, $\text{GaPO}_4 \cdot 2\text{H}_2\text{O}$	8m	34
Copper hydroxide carbonate, azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$	10	30	Gallium phosphate (α -quartz type), GaPO_4	8	27
Copper hydroxide carbonate (malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$	10	31	Germanium, Ge	1	18
Copper(I) iodide (marchite), CuI	4	38	Germanium iodide, GeI_2	4m	58
Copper(I) oxide (cuprite), Cu_2O	2	23	Germanium(IV) iodide, GeI_4	5	25
Copper(II) oxide (tenorite), CuO	1	49	Germanium oxide, GeO_2 (hexagonal) (low form)	1	51
Copper phosphate, alpha $\text{Cu}_3\text{P}_2\text{O}_7$	7m	113	Germanium oxide, GeO_2 (tetragonal) (high form)	8	28
Copper sulfate (chalcocyanite), CuSO_4	3m	29	Gold, Au	1	33
Copper(II) sulfide (covellite), CuS	4	13	Gold antimony 1:2 (aurostibite), AuSb_2	7	18
Copper uranium oxide, CuUO_4	10m	93	Gold(I) cyanide, AuCN	10	33
Dysprosium antimony, DySb	4m	41	Gold potassium cyanide, $\text{AuK}(\text{CN})_2$	8m	36
Dysprosium arsenate, DyAsO_4	3m	30	Gold tin, 1:1 AuSn	7	19
Dysprosium arsenide, DyAs	4m	53	Gold titanium 1:3, AuTi_3	6m	17
Dysprosium bismuth, DyBi	4m	47	Hafnium, Hf	3	18
Dysprosium gallium oxide, $\text{Dy}_3\text{Ga}_2(\text{GaO}_4)_3$	2m	15	Holmium arsenate, HoAsO_4	3m	34
Dysprosium gold, DyAu	5m	66	Holmium bismuth, HoBi	4m	48
Dysprosium nitride, DyN	4m	53	Holmium fluoride, HoF_3	10m	23
Dysprosium oxide, Dy_2O_3	9	30	Holmium gold, HoAu	5m	68
Dysprosium silver, DyAg	5m	66	Holmium nitride, HoN	4m	58
Dysprosium telluride, DyTe	4m	54	Holmium oxide, Ho_2O_3	9	32
Dysprosium vanadium oxide, DyVO_4	4m	15	Holmium selenide, HoSe	4m	59
Erbium antimony, ErSb	4m	41	Holmium silver, HoAg	5m	68
Erbium arsenate, ErAsO_4	3m	31	Holmium vanadium oxide, HoVO_4	4m	18
Erbium arsenide, ErAs	4m	54	Hydrogen borate, beta HBO_2	9m	71
Erbium bismuth, ErBi	4m	47	Hydrogen iodate, HIO_3	5	28
Erbium gallium oxide, $\text{Er}_3\text{Ga}_2(\text{GaO}_4)_3$	1m	12	Hydrogen iodate, HI_3O_8	8m	104
Erbium manganese oxide, ErMnO_3	2m	16	Indium, In	3	12
Erbium nitride, ErN	4m	55	Indium antimony, InSb	4	73
Erbium oxide, Er_2O_3	8	25	Indium arsenide, InAs	3m	35
Erbium phosphate, ErPO_4	9	31	Indium oxide, In_2O_3	5	26
Erbium silver, ErAg	5m	67	Indium phosphate, InPO_4	8	29
Erbium telluride, ErTe	4m	55	Indium sulfide, In_2S_3	11m	30
Erbium vanadium oxide, ErVO_4	5m	29	Iodine, I_2	3	16
Europium arsenate, EuAsO_4	3m	32	Iridium, Ir	4	9
Europium(III) chloride, EuCl_3	1m	13	Iridium oxide, IrO_2	4m	19
Europium gallium oxide, $\text{Eu}_3\text{Ga}_2(\text{GaO}_4)_3$	2m	17	Iridium titanium 1:3, IrTi_3	6m	20
Europium nitride, EuN	4m	56	Iron, alpha Fe	4	3
Europium oxide, EuO	4m	56	Iron arsenide, FeAs	1m	19
Europium oxychloride, EuOCl	1m	13	Iron arsenide (loellingite), FeAs_2	10	34
Europium phosphate, EuPO_4	11m	26	Iron bromide, FeBr_3	4m	59
Europium(III) vanadium oxide, EuVO_4	4m	16	Iron chloride hydrate, $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$	11m	32
Gadolinium antimony, GdSb	4m	42	Iron fluoride hydrate, $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$	11m	90
Gadolinium arsenate, GdAsO_4	4m	17	Iron hydroxide sulfate hydrate, butlerite, $\text{Fe}(\text{OH})\text{SO}_4 \cdot 2\text{H}_2\text{O}$	10m	95
Gadolinium arsenide, GdAs	4m	57	Iron iodide, FeI_2	4m	60
Gadolinium chloride hydrate, $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$	7m	118	Iron(II,III) oxide (magnetite), Fe_3O_4	5m	31
Gadolinium fluoride, GdF_3	1m	14	Iron sulfate hydrate (melanterite), $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$	8m	38
			Iron sulfide (pyrite), FeS_2	5	29
			Lanthanum antimony, LaSb	4m	42
			Lanthanum arsenate, LaAsO_4	3m	36
			Lanthanum arsenide, LaAs	4m	60
			Lanthanum bismuth, LaBi	4m	48

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Lanthanum cadmium, LaCd	5m	63	Lithium phosphate, high form, Li_3PO_4	3m	39
Lanthanum chloride, LaCl_3	1m	20	Lithium rubidium fluoride, LiRbF_6	7m	128
Lanthanum fluoride, LaF_3	7	21	Lithium selenide, Li_2Se	10m	100
Lanthanum niobium titanium oxide, LaNbTiO_6	3m	37	Lithium sodium aluminum fluoride, cryolithionite, $\text{Li}_3\text{Na}_3\text{Al}_3\text{F}_{12}$	9m	23
Lanthanum nitrate hydrate, $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$	8m	40	Lithium sodium sulfate, LiNaSO_4	6m	24
Lanthanum nitride, LaN	4m	61	Lithium sulfate, Li_2SO_4	6m	26
Lanthanum oxide, La_2O_3	3	33	Lithium sulfate hydrate, $\text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$	4m	22
Lanthanum oxychloride, LaOCl	7	22	Lithium sulfide, Li_2S	10m	101
Lanthanum phosphide, LaP	5m	69	Lithium telluride, Li_2Te	10m	102
Lanthanum selenide, LaSe	4m	61	Lithium tungsten oxide, Li_2WO_4 (trigonal) ...	1m	25
Lanthanum zinc, LaZn	5m	70	Lithium tungsten oxide hydrate, $\text{Li}_2\text{WO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$	2m	20
Lead, Pb	1	34	Lithium uranium fluoride, LiUF_6	7m	131
Lead borate, PbB_4O_7	4m	19	Lutetium arsenate, LuAsO_4	5m	36
Lead bromide, PbBr_2	2	47	Lutetium gallium oxide, $\text{Lu}_3\text{Ga}_2(\text{GaO}_4)_3$	2m	22
Lead bromide chloride, PbBrCl	11m	33	Lutetium manganese oxide, LuMnO_3	2m	23
Lead bromide fluoride, PbBrF	10m	25	Lutetium nitride, LuN	4m	62
Lead carbonate (cerussite), PbCO_3	2	56	Lutetium oxide, Lu_2O_3	1m	27
Lead chloride (cotunnite), PbCl_2	2	45	Lutetium vanadium oxide, LuVO_4	5m	37
Lead chloride fluoride (matlockite), PbClF	1	76	Magnesium, Mg	1	10
Lead fluoride, alpha PbF_2 (orthorhombic)	5	31	Magnesium aluminum oxide (spinel), MgAl_2O_4 (revised)	9m	25
Lead fluoride, beta PbF_2 (cubic)	5	33	Magnesium aluminum silicate (pyrope), $\text{Mg}_3\text{Al}_2(\text{SiO}_4)_3$	4m	24
Lead fluoride iodide, PbFI	10m	26	Magnesium aluminum silicate (low cordi- erite), $\text{Mg}_3\text{Al}_2\text{Si}_5\text{O}_{18}$ (orthorhombic)	1m	28
Lead hydroxide phosphate, $\text{Pb}_5(\text{PO}_4)_3\text{OH}$	8	33	Magnesium aluminum silicate (high cordi- erite), $\text{Mg}_3\text{Al}_2\text{Si}_5\text{O}_{18}$ (hexagonal)	1m	29
Lead(II) iodide, PbI_2	5	34	Magnesium ammonium phosphate hydrate, (struvite), $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$	3m	41
Lead molybdenum oxide (wulfenite), PbMoO_4	7	23	Magnesium borate, $\text{Mg}_2\text{B}_2\text{O}_5$ (triclinic)	4m	25
Lead nitrate, $\text{Pb}(\text{NO}_3)_2$	5	36	Magnesium bromide, MgBr_2	4m	62
Lead oxide (litharge), PbO (red, tetragonal) ..	2	30	Magnesium bromide hydrate, $\text{MgBr}_2 \cdot 6\text{H}_2\text{O}$	11m	35
Lead oxide (massicot), PbO (yellow, ortho- rhombic)	2	32	Magnesium carbonate (magnesite), MgCO_3	7	28
Lead(II, III) oxide (minium), Pb_3O_4	8	32	Magnesium cerium MgCe	5m	65
Lead oxide sulfate, $\text{Pb}_5\text{O}_4\text{SO}_4$	10m	27	Magnesium cerium nitrate hydrate, $\text{Mg}_3\text{Ce}_2(\text{NO}_3)_{12} \cdot 24\text{H}_2\text{O}$	10	20
Lead oxybromide, $\text{Pb}_3\text{O}_4\text{Br}_2$	5m	32	Magnesium chlorate hydrate, $\text{Mg}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$	7m	30
Lead selenide (clausthalite), PbSe	5	38	Magnesium chloride (chloromagnesite), MgCl_2	11m	94
Lead sulfate (anglesite), PbSO_4	3	67	Magnesium chloride hydrate, $\text{MgCl}_2 \cdot 12\text{H}_2\text{O}$..	7m	135
Lead sulfide (galena), PbS	2	18	Magnesium chloride hydrate (bischofite), $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$	11m	37
Lead tin oxide, Pb_2SnO_4	10m	29	Magnesium chromium oxide (picrochromite), MgCr_2O_4	9	34
Lead titanium oxide, PbTiO_3	5	39	Magnesium fluoride (sellaite), MgF_2	4	33
Lead tungsten oxide (stolzite), PbWO_4 (tetragonal) (revised)	5m	34	Magnesium fluoride silicate (humite), $\text{Mg}_7\text{F}_2(\text{SiO}_4)_3$	1m	30
Lead uranium oxide, Pb_3UO_6	8m	109	Magnesium fluoride silicate (norbergite), $\text{Mg}_3\text{F}_2\text{SiO}_4$	10	39
Lutetium manganese oxide, LuMnO_3	2m	23	Magnesium gallium oxide, MgGa_2O_4	10	36
Lithium aluminum, Li_9Al_4	10m	98	Magnesium germanium oxide, Mg_2GeO_4 (cubic)	10	37
Lithium aluminum fluoride, alpha Li_3AlF_6	8m	111	Magnesium germanium oxide, Mg_2GeO_4 (ortho- rhombic)	10	38
Lithium arsenate, Li_3AsO_4	2m	19	Magnesium gold, MgAu	6m	83
Lithium azide, LiN_3	8m	113	Magnesium hydrogen phosphate hydrate, newberyite, $\text{MgHPO}_4 \cdot 3\text{H}_2\text{O}$	7m	139
Lithium barium fluoride, LiBaF_3	5m	35	Magnesium hydroxide (brucite), $\text{Mg}(\text{OH})_2$	6	30
Lithium beryllium fluoride, Li_2BeF_4	7m	126	Magnesium iron hydroxide carbonate hydrate, pyroaurite, $\text{Mg}_2\text{Fe}_2(\text{OH})_{16}\text{CO}_3 \cdot 4\text{H}_2\text{O}$, phase II	10m	104
Lithium borate, $\text{Li}_2\text{B}_4\text{O}_7$	8m	114	Magnesium iron hydroxide carbonate hydrate, sjögrenite, $\text{Mg}_2\text{Fe}_2(\text{OH})_{16}\text{CO}_3 \cdot 4\text{H}_2\text{O}$, phase I	10m	103
Lithium bromide, LiBr	4	30	Magnesium lanthanum, MgLa	5m	69
Lithium carbonate, Li_2CO_3	8m	42	Magnesium lanthanum nitrate hydrate, $\text{Mg}_3\text{La}_2(\text{NO}_3)_{12} \cdot 24\text{H}_2\text{O}$	1m	22
Lithium chlorate hydrate, $\text{LiClO}_4 \cdot 3\text{H}_2\text{O}$	8	34			
Lithium chloride, LiCl	1	62			
Lithium fluoride, LiF	1	61			
Lithium gallium oxide, LiGaO_2	10m	31			
Lithium hydroxide hydrate, $\text{LiOH} \cdot \text{H}_2\text{O}$	11m	92			
Lithium iodate, LiIO_3	7	26			
Lithium iodate, LiIO_3 (tetragonal)	10m	33			
Lithium molybdenum oxide, Li_2MoO_4 (trigonal)	1m	23			
Lithium niobium oxide, LiNbO_3	6m	22			
Lithium nitrate, LiNO_3	7	27			
Lithium oxide, Li_2O	1m	25			
Lithium phosphate hydrate, $\text{Li}_3\text{P}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$...	2m	20			

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Magnesium manganese oxide, MgMn_2O_4	10m	35	Molybdenum oxide (molybdate), MoO_3	3	30
Magnesium mercury, MgHg	6m	84	Molybdenum sulfide (molybenite), MoS_2	5	47
Magnesium molybdenum oxide, MgMoO_4	7m	28	Neodymium antimony, NdSb	4m	43
Magnesium nickel oxide, MgNiO_2	10m	36	Neodymium arsenate, NdAsO_4	4m	28
Magnesium oxide (periclase), MgO	1	37	Neodymium arsenide, NdAs	4m	64
Magnesium phosphate, alpha $\text{Mg}_2\text{P}_2\text{O}_7$	9m	73	Neodymium bismuth, NdBi	4m	49
Magnesium selenide, MgSe	5m	70	Neodymium borate, NdBO_3	1m	32
Magnesium selenite hydrate, $\text{MgSeO}_3 \cdot 6\text{H}_2\text{O}$	8m	116	Neodymium chloride, NdCl_3	1m	33
Magnesium silicate, enstatite, MgSiO_3	6	32	Neodymium fluoride, NdF_3	8	36
Magnesium silicate (forsterite), Mg_2SiO_4	1	83	Neodymium gallium oxide, $\text{Nd}_3\text{Ga}_2(\text{GaO}_4)_3$	1m	34
Magnesium sulfate hydrate (epsomite), $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$	7	30	Neodymium oxide, Nd_2O_3	4	26
Magnesium sulfide, MgS	7	31	Neodymium oxychloride, NdOCl	8	37
Magnesium sulfite hydrate, $\text{MgSO}_3 \cdot 6\text{H}_2\text{O}$	9m	26	Neodymium phosphate, NdPO_4	11m	40
Magnesium titanium oxide (geikielite), MgTiO_3	5	43	Neodymium selenide, NdSe	5m	71
Magnesium tin, Mg_2Sn	5	41	Neodymium silver, NdAg	5m	71
Magnesium tin oxide, Mg_2SnO_4	10m	37	Neodymium vanadium oxide, NdVO_4	4m	30
Magnesium tungsten oxide, MgWO_4	1	84	Neptunium nitride, NpN	4m	64
Manganese, alpha, Mn	7m	142	Nickel, Ni	1	13
Manganese aluminum oxide (galaxite), MnAl_2O_4	9	35	Nickel aluminum, NiAl	6m	82
Manganese bromide, MnBr_2	4m	63	Nickel aluminum oxide, NiAl_2O_4	9	42
Manganese(II) carbonate (rhodochrosite), MnCO_3	7	32	Nickel arsenide 1:2 (rammelsbergite), NiAs_2	10	42
Manganese chloride hydrate, $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$	11m	38	Nickel arsenic sulfide (gersdorffite), NiAsS	1m	35
Manganese chloride (scacchite), MnCl_2	8m	43	Nickel bromide, NiBr_2	10m	119
Manganese chloride hydrate, $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$	9m	28	Nickel(II) carbonate, NiCO_3 (trigonal)	1m	36
Manganese cobalt oxide, MnCo_2O_4	9m	30	Nickel chloride, NiCl_2	9m	81
Manganese fluoride, MnF_2	10m	105	Nickel chloride hydrate, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	11m	42
Manganese iodide, MnI_2	4m	63	Nickel fluoride, NiF_2	10m	121
Manganese iron oxide (jacobsonite), MnFe_2O_4	9	36	Nickel fluoride hydrate, $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$	11m	43
Manganese oxide (hausmannite), Mn_3O_4	10m	38	Nickel gallium oxide, NiGa_2O_4	10	45
Manganese oxide (partridgeite), alpha Mn_2O_3 (revised)	11m	95	Nickel germanium oxide, Ni_2GeO_4	9	43
Manganese oxide (pyrolusite), beta, MnO_2	10m	39	Nickel iron oxide (trevorite), NiFe_2O_4	10	44
Manganese oxide hydroxide, groutite, alpha MnOOH	11m	97	Nickel(II) oxide (bunsenite), NiO	1	47
Manganese(II) oxide (manganosite), MnO	5	45	Nickel phosphide, Ni_3P_2	9m	83
Manganese selenide, MnSe	10	41	Nickel silicon fluoride hydrate, $\text{NiSiF}_6 \cdot 6\text{H}_2\text{O}$	8	38
Manganese sulfide (alabandite), alpha MnS	4	11	Nickel sulfate, NiSO_4	2m	26
Manganese(II) tungsten oxide (huebnerite), MnWO_4	2m	24	Nickel sulfate hydrate (retgersite), $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$	7	36
Manganese vanadium oxide, $\text{Mn}_2\text{V}_2\text{O}_7$	9m	75	Nickel sulfide, millerite, NiS	1m	37
Mercury amide chloride, HgNH_2Cl	10m	40	Nickel tungsten oxide, NiWO_4	2m	27
Mercury ammine chloride, $\text{Hg}(\text{NH}_3)_2\text{Cl}_2$	11m	39	Niobium gold 3:1, Nb_3Au	6m	16
Mercury bromate, $\text{Hg}(\text{BrO}_3)_2$	10m	107	Niobium iridium 3:1, Nb_3Ir	6m	19
Mercury bromide, HgBr_2	10m	110	Niobium osmium 3:1, Nb_3Os	6m	30
Mercury(I) bromide, Hg_2Br_2	7	33	Niobium oxychloride, NbOCl_3	7m	148
Mercury(I) chloride (calomel), Hg_2Cl_2	1	72	Niobium platinum 3:1, Nb_3Pt	6m	31
Mercury(II) chloride, HgCl_2	1	73	Niobium silicide, NbSi_2	8	39
Mercury chloride sulfide, alpha $\text{Hg}_2\text{Cl}_2\text{S}_2$	8m	118	Osmium, Os	4	8
Mercury(II) cyanide, $\text{Hg}(\text{CN})_2$	6	35	Osmium titanium, OsTi	6m	85
Mercury(II) fluoride, HgF_2	2m	25	Palladium, Pd	1	21
Mercury(I) iodide, HgI_2	4	49	Palladium hydride, $\text{PdH}_{0.706}$	5m	72
Mercury iodide, HgI_2 (tetragonal) (revised)	7m	32	Palladium oxide, PdO	4	27
Mercury(II) oxide (montroydite) HgO (revised)	9	39	Phosphorus bromide, PBr_3	7m	150
Mercury(II) selenide (tiemannite), HgSe	7	35	Phosphorus oxide (stable form I), P_2O_5 , (orthorhombic)	9m	86
Mercury(II) sulfide (cinnabar), HgS (hex- agonal)	4	17	Phosphorus oxide (stable form II), P_2O_5 , (orthorhombic)	9m	88
Mercury(II) sulfide (metacinnabar), HgS (cubic)	4	21	Phosphorus oxide (metastable form), P_4O_{10} , (rhombohedral)	9m	91
Molybdenum, Mo	1	20	Platinum, Pt	1	31
Molybdenum arsenide, Mo_3As_4	10m	115	Platinum titanium 1:3, PtTi_3	6m	33
Molybdenum osmium 3:1, Mo_3Os	6m	28	Plutonium arsenide, PuAs	4m	65
			Plutonium phosphide, PuP	4m	65
			Plutonium telluride, PuTe	4m	66
			Potassium aluminum sulfate, $\text{KAl}(\text{SO}_4)_2$	9m	31
			Potassium aluminum sulfate hydrate, (alum), $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	36

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Potassium barium nickel nitrite, K ₂ BaNi(NO ₂) ₆	9m	32	Potassium molybdenum oxide phosphate hydrate, K ₂ (MoO ₃) ₁₂ PO ₄ ·4H ₂ O	8	43
Potassium borohydride, KBH ₄	9	44	Potassium nickel fluoride, KNiF ₃	7m	42
Potassium bromate, KBrO ₃	7	38	Potassium nickel fluoride, K ₂ NiF ₄	10m	45
Potassium bromide, KBr	1	66	Potassium nickel (II) sulfate, K ₂ Ni ₂ (SO ₄) ₃	6m	46
Potassium bromide chloride, KBr _{0.5} Cl _{0.5}	8m	46	Potassium niobium fluoride, K ₂ NbF ₇	8m	120
Potassium bromide iodide, KBr _{0.33} I _{0.67}	11m	44	Potassium nitrate (niter), KNO ₃	3	58
Potassium bromide iodide, KBr _{0.67} I _{0.33}	11m	45	Potassium nitrite, KNO ₂	9m	38
Potassium cadmium fluoride, KCdF ₃	8m	47	Potassium nitroso ruthenium chloride, K ₂ (NO)RuCl ₅	2m	29
Potassium cadmium sulfate, K ₂ Cd ₂ (SO ₄) ₃	7m	34	Potassium oxide, K ₂ O	10m	125
Potassium calcium carbonate (fairchildite), K ₂ Ca(CO ₃) ₂	8m	48	Potassium platinum bromide, K ₂ PtBr ₆	8	40
Potassium calcium chloride (chlorocalcite), KCaCl ₃	7m	36	Potassium platinum chloride, K ₂ PtCl ₆	5	49
Potassium calcium fluoride, KCaF ₃	8m	49	Potassium platinum fluoride, K ₂ PtF ₆	6	42
Potassium calcium magnesium sulfate, K ₂ CaMg(SO ₄) ₃	7m	37	Potassium rhenium chloride, K ₂ ReCl ₆	2m	28
Potassium calcium nickel nitrite, K ₂ CaNi(NO ₂) ₆	9m	33	Potassium rhenium oxide, KReO ₄	8	41
Potassium calcium sulfate, K ₂ Ca ₂ (SO ₄) ₃	7m	39	Potassium rubidium chloride, Rb _{0.5} K _{0.5} Cl ...	8m	76
Potassium chlorate, KClO ₃	3m	42	Potassium ruthenium chloride, K ₂ RuCl ₆	10	46
Potassium chlorate, KClO ₄	6	43	Potassium ruthenium oxide chloride hydrate, K ₂ Ru ₂ OCl ₁₀ ·H ₂ O	10	47
Potassium chloride (sylvite), KCl	1	65	Potassium selenate, K ₂ SeO ₄	9m	41
Potassium chromium oxide, K ₃ CrO ₄	3m	44	Potassium selenide, K ₂ Se	10m	126
Potassium chromium sulfate hydrate, KCr(SO ₄) ₂ ·12H ₂ O	6	39	Potassium selenium bromide, K ₂ SeBr ₆	8	41
Potassium cobalt(II) fluoride, KCoF ₃	6m	37	Potassium silicon fluoride (hieratite), K ₂ SiF ₆	5	50
Potassium cobalt fluoride, K ₂ CoF ₄	11m	46	Potassium silver cyanide, KAg(CN) ₂	8m	78
Potassium cobalt nitrite, K ₃ Co(NO ₂) ₆	9	45	Potassium sodium aluminum fluoride (elpasolite), K ₂ NaAlF ₆	9m	43
Potassium cobalt (II) sulfate, K ₂ Co ₂ (SO ₄) ₃ ...	6m	35	Potassium sodium sulfate, KNaSO ₄	6m	50
Potassium copper chloride, KCuCl ₃	7m	41	Potassium sodium sulfate, K _{0.67} Na _{1.33} SO ₄	6m	48
Potassium copper chloride hydrate (mitscherlichite), K ₂ CuCl ₄ ·2H ₂ O	9m	34	Potassium sodium sulfate (aphthalite), K ₃ Na(SO ₄) ₂	6m	52
Potassium copper(II) fluoride, KCuF ₃	6m	38	Potassium sulfate, K ₂ S ₂ O ₇	9m	99
Potassium cyanate, KCNO	7	39	Potassium sulfate (arcanite), K ₂ SO ₄	3	62
Potassium cyanide, KCN	1	77	Potassium sulfide, K ₂ S	10m	127
Potassium fluoride, KF	1	64	Potassium telluride, K ₂ Te	10m	128
Potassium germanium fluoride, K ₂ GeF ₆	6	41	Potassium thiocyanate, KCNS	8	44
Potassium hydrogen arsenate, KH ₂ AsO ₄	1m	38	Potassium tin chloride, K ₂ SnCl ₆	6	38
Potassium hydrogen phosphate, KH ₂ PO ₄	3	69	Potassium titanium fluoride, K ₂ TiF ₆	7	40
Potassium hydroxide, KOH at 300 °C	4m	66	Potassium tungsten oxide, K ₂ WO ₄	11m	47
Potassium iodide, KI	1	68	Potassium vanadium oxide, KV ₃ O ₅	8m	56
Potassium iodate, KIO ₄	7	41	Potassium zinc bromide hydrate, KZnBr ₃ ·2H ₂ O	11m	104
Potassium iron cyanide, K ₃ Fe(CN) ₆	9m	35	Potassium zinc fluoride, KZnF ₃	5	51
Potassium iron fluoride, K ₃ FeF ₆	9m	37	Potassium zinc fluoride, K ₂ ZnF ₄	10m	46
Potassium iron(II) fluoride, KFeF ₃	6m	39	Potassium zinc iodide hydrate, KZnI ₃ ·2H ₂ O ..	11m	107
Potassium lithium sulfate, KLiSO ₄	3m	43	Potassium zinc sulfate, K ₂ Zn ₂ (SO ₄) ₃	6m	54
Potassium magnesium chloride hydrate (carnallite), KMgCl ₃ ·6H ₂ O	8m	50	Potassium zinc sulfate hydrate, K ₂ Zn(SO ₄) ₂ ·6H ₂ O	7m	43
Potassium magnesium chromium oxide, K ₂ Mg ₂ (CrO ₄) ₃	8m	52	Potassium zinc vanadium oxide hydrate, K ₂ Zn ₂ V ₁₀ O ₂₈ ·16H ₂ O	3m	45
Potassium magnesium fluoride, KMgF ₃	6m	42	Potassium zirconium fluoride, K ₂ ZrF ₇	9	46
Potassium magnesium fluoride, K ₂ MgF ₄	10m	42	Praseodymium antimony, PrSb	4m	43
Potassium magnesium selenate hydrate, K ₂ Mg(SeO ₄) ₂ ·6H ₂ O	10m	43	Praseodymium arsenate, PrAsO ₄	4m	32
Potassium magnesium sulfate (langbeinite), K ₂ Mg ₂ (SO ₄) ₃	6m	40	Praseodymium arsenide, PrAs	4m	67
Potassium magnesium sulfate hydrate (picromerite), K ₂ Mg(SO ₄) ₂ ·6H ₂ O	8m	54	Praseodymium bismuth, PrBi	4m	49
Potassium manganese (II) fluoride, KMnF ₃ ...	6m	45	Praseodymium cadmium, PrCd	5m	64
Potassium manganese oxide, KMnO ₄	7	42	Praseodymium chloride, PrCl ₃	1m	39
Potassium manganese (II) sulfate (manganolangbeinite), K ₂ Mn ₂ (SO ₄) ₃	6m	43	Praseodymium fluoride, PrF ₃	5	52
			Praseodymium oxychloride, PrOCl	9	47
			Praseodymium sulfide, PrS	4m	67
			Praseodymium vanadium oxide, PrVO ₄	5m	40
			Praseodymium zinc, PrZn	5m	72
			Rhenium, Re	2	13
			Rhodium, Rh	3	9
			Rubidium aluminum sulfate hydrate, RbAl(SO ₄) ₂ ·12H ₂ O	6	44

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Rubidium amide, RbNH_2	5m	73	Samarium oxychloride, SmOCl	1m	43
Rubidium bromate, RbBrO_3	8	45	Samarium silver, SmAg	5m	73
Rubidium bromide, RbBr	7	43	Samarium tin oxide, $\text{Sm}_3\text{Sn}_2\text{O}_7$	8m	77
Rubidium cadmium chloride, high form, RbCdCl_3 (tetragonal)	5m	43	Samarium vanadium oxide, SmVO_4	5m	47
Rubidium cadmium chloride, low form, RbCdCl_3 (orthorhombic)	5m	41	Scandium antimony, ScSb	4m	44
Rubidium cadmium sulfate, $\text{Rb}_2\text{Cd}_2(\text{SO}_4)_3$	7m	45	Scandium arsenate, ScAsO_4	4m	35
Rubidium calcium chloride, RbCaCl_2	7m	47	Scandium arsenide, ScAs	4m	68
Rubidium calcium fluoride, RbCaF_3	8m	57	Scandium oxide, Sc_2O_3	3	27
Rubidium calcium sulfate, $\text{Rb}_2\text{Ca}_2(\text{SO}_4)_3$	7m	48	Scandium phosphate, ScPO_4	8	50
Rubidium chlorate, RbClO_3	8	47	Scandium silicate (thortveitite), $\text{Sc}_2\text{Si}_2\text{O}_7$	7m	58
Rubidium chlorate, RbClO_4	2m	30	Selenium, Se	5	54
Rubidium chloride, RbCl	4	41	Selenium oxide (selenolite), SeO , (revised)	7m	60
Rubidium chromium oxide, Rb_2CrO_4	3m	46	Silicon, Si	2	6
Rubidium chromium sulfate hydrate, $\text{RbCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	6	47	Silicon oxide, (alpha or low cristobalite), SiO_2 (tetragonal) (revised)	10	48
Rubidium cobalt (II) chloride, RbCoCl_2	6m	57	Silicon oxide (alpha or low quartz), SiO_2 (hexagonal)	3	24
Rubidium cobalt fluoride, RbCoF_3	8m	58	Silicon oxide (beta or high cristobalite), SiO_2 (cubic)	1	42
Rubidium cobalt sulfate, $\text{Rb}_2\text{Co}_2(\text{SO}_4)_3$	8m	59	Silver, Ag	1	23
Rubidium copper chloride hydrate, $\text{Rb}_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$	10m	47	Silver, Ag (reference standard)	8m	2
Rubidium copper sulfate hydrate, $\text{Rb}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	61	Silver antimony sulfide, AgSbS_2 (cubic)	5m	48
Rubidium fluoride, RbF	8m	63	Silver antimony sulfide (miargyrite), AgSbS_2 (monoclinic)	5m	49
Rubidium iodate, RbIO_4	2m	31	Silver antimony sulfide (pyrargyrite), Ag_3SbS_3 (trigonal)	5m	51
Rubidium iodide, RbI	4	43	Silver antimony telluride, AgSbTe_2	3m	47
Rubidium iron sulfate hydrate, $\text{Rb}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	64	Silver arsenate, Ag_3AsO_4	5	56
Rubidium magnesium chromium oxide, $\text{Rb}_2\text{Mg}_2(\text{CrO}_4)_3$	8m	66	Silver arsenic sulfide, xanthoconite, Ag_3AsS_3	8m	126
Rubidium magnesium chromium oxide hydrate, $\text{Rb}_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	68	Silver bromate, AgBrO_3	5	57
Rubidium magnesium sulfate, $\text{Rb}_2\text{Mg}_2(\text{SO}_4)_3$	7m	50	Silver bromide (bromyrite), AgBr	4	46
Rubidium magnesium sulfate hydrate, $\text{Rb}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	70	Silver carbonate, Ag_2CO_3	1m	44
Rubidium manganese (II) fluoride, RbMnF_3	5m	44	Silver chlorate, AgClO_3	7	44
Rubidium manganese sulfate, $\text{Rb}_2\text{Mn}_2(\text{SO}_4)_3$	7m	52	Silver chloride, (cerargyrite), AgCl	4	44
Rubidium nickel (II) chloride, RbNiCl_2	6m	58	Silver cyanide, AgCN	9m	48
Rubidium nickel sulfate, $\text{Rb}_2\text{Ni}_2(\text{SO}_4)_3$	8m	72	Silver fluoride, AgF	5m	53
Rubidium nickel sulfate hydrate, $\text{Rb}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	8m	74	Silver iodate, AgIO_4	9	49
Rubidium nitrate, RbNO_3 (trigonal)	5m	45	Silver iodide (iodyrite), AgI (hexagonal)	8	51
Rubidium platinum chloride, Rb_2PtCl_6	5	53	Silver iodide, gamma, AgI (cubic)	9	48
Rubidium platinum fluoride, Rb_2PtF_6	6	48	Silver manganese oxide, AgMnO_4	7m	155
Rubidium selenate, Rb_2SeO_4	9m	44	Silver molybdenum oxide, Ag_2MoO_4	7	45
Rubidium silicon fluoride, Rb_2SiF_6	6	49	Silver nitrate, AgNO_3	5	59
Rubidium strontium chloride, RbSrCl_2	7m	54	Silver nitrite, AgNO_2	5	60
Rubidium sulfate, Rb_2SO_4	8	48	Silver oxide, Ag_2O	1m	45
Rubidium tellurium bromide, Rb_2TeBr_6	8	46	Silver(II) oxide nitrate, $\text{Ag}_2\text{O}_2\text{NO}_3$	4	61
Rubidium tellurium chloride, Rb_2TeCl_6	8	48	Silver phosphate, Ag_3PO_4	5	62
Rubidium tin chloride, Rb_2SnCl_6	6	46	Silver rhenium oxide, AgReO_4	8	53
Rubidium zinc fluoride, RbZnF_3	7m	57	Silver selenate, Ag_2SeO_4	2m	32
Rubidium zinc sulfate hydrate, $\text{Rb}_2\text{Zn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	7m	55	Silver sodium chloride, $\text{Ag}_{0.5}\text{Na}_{0.5}\text{Cl}$	8m	79
Ruthenium, Ru	4	5	Silver sulfate, Ag_2SO_4	7	46
Ruthenium titanium, RuTi	6m	86	Silver sulfide (argentite), Ag_2S	10	51
Samarium arsenate, SmAsO_4	4m	33	Sodium, Na	9m	105
Samarium arsenide, SmAs	4m	68	Sodium aluminum chloride silicate, sodalite, $\text{Na}_4\text{Al}_6\text{Cl}_2(\text{SiO}_4)_6$	7m	158
Samarium chloride, SmCl_3	1m	40	Sodium azide, alpha, NaN_3 , at -90 to -100°C	8m	129
Samarium fluoride, SmF_3	1m	41	Sodium azide, beta NaN_3	8m	130
Samarium gallium oxide, $\text{Sm}_3\text{Ga}_2(\text{GaO}_4)_3$	1m	42	Sodium beryllium calcium fluoride silicate, leucophanite, $\text{NaBeCaF}_2\text{Si}_2\text{O}_6$	8m	138
Samarium oxide, Sm_2O_3 (cubic)	4m	34	Sodium borate, $\text{Na}_2\text{B}_4\text{O}_{10}$	7m	160
			Sodium boron hydride, NaBH_4	9	51
			Sodium bromate, NaBrO_3	5	65
			Sodium bromide, NaBr	3	47
			Sodium bromide chloride, $\text{NaBr}_{.33}\text{Cl}_{.67}$	11m	49
			Sodium bromide chloride, $\text{NaBr}_{.67}\text{Cl}_{.33}$	11m	50
			Sodium calcium aluminum fluoride hydrate, thomsenolite, $\text{NaCaAlF}_6 \cdot \text{H}_2\text{O}$	8m	132

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Sodium calcium beryllium aluminum fluorosilicate, meliphanite, (Na _{0.63} Ca _{1.37})Be(Al _{0.13} Si _{1.87}) (O _{6.25} F _{0.75})	8m	135	Sodium nitrite, NaNO ₂	4	62
Sodium calcium carbonate hydrate, pirssonite, Na ₂ Ca (CO ₃) ₂ ·2H ₂ O	9m	106	Sodium oxide, Na ₂ O	10m	134
Sodium calcium silicate, Na ₂ CaSiO ₄	10m	48	Sodium phosphate, Na ₃ P ₃ O ₉	3m	49
Sodium calcium sulfate (glauberite), Na ₂ Ca(SO ₄) ₂	6m	59	Sodium phosphate hydrate, Na ₃ P ₃ O ₉ ·H ₂ O	3m	50
Sodium carbonate hydrate (thermonatrite), Na ₂ CO ₃ ·H ₂ O	8	54	Sodium phosphate hydrate, alpha Na ₄ P ₄ O ₁₂ ·4H ₂ O (monoclinic)	10	52
Sodium carbonate sulfate, Na ₄ CO ₃ SO ₄	11m	51	Sodium phosphate hydrate, beta Na ₄ P ₄ O ₁₂ ·4H ₂ O (triclinic)	2m	35
Sodium carbonate sulfate (burkeite), Na ₆ CO ₃ (SO ₄) ₂	11m	52	Sodium phosphate hydrate, Na ₆ P ₆ O ₁₈ ·6H ₂ O	5m	54
Sodium carbonate sulfate, Na ₄ CO ₃ (SO ₄) ₂	11m	53	Sodium praseodymium fluoride silicate, (Na ₂ Pr ₆)F ₂ (SiO ₄) ₆	7m	68
Sodium carbonate sulfate, Na ₆ (CO ₃) ₂ SO ₄	11m	54	Sodium selenate, Na ₂ SeO ₄	9m	55
Sodium chlorate, NaClO ₃	3	51	Sodium selenide, Na ₂ Se	10m	135
Sodium chlorate, NaClO ₄ orthorhombic	7	49	Sodium silicate, alpha (III), Na ₂ Si ₂ O ₅	8m	141
Sodium chloride (halite), NaCl	2	41	Sodium silicate, beta Na ₂ Si ₂ O ₅	10m	136
Sodium chromium oxide, Na ₂ CrO ₄	9m	48	Sodium sulfate (thenardite), Na ₂ SO ₄	2	59
Sodium chromium oxide hydrate, Na ₂ Cr ₂ O ₇ ·2H ₂ O	7m	62	Sodium sulfate, Na ₂ SO ₄	11m	57
Sodium chromium oxide hydrate, Na ₂ CrO ₄ ·4H ₂ O	9m	50	Sodium sulfide, Na ₂ S	10m	140
Sodium chromium oxide sulfate, Na ₄ (CrO ₄)(SO ₄)	11m	55	Sodium sulfite, Na ₂ SO ₃	3	60
Sodium cobalt(II) sulfate hydrate, Na ₂ Co(SO ₄) ₂ ·4H ₂ O	6m	61	Sodium telluride, Na ₂ Te	10m	141
Sodium cyanate, NaCNO	2m	33	Sodium tin fluoride, NaSn ₃ F ₄	7m	166
Sodium cyanide, NaCN (cubic)	1	78	Sodium tungsten oxide, Na ₂ WO ₄	1m	47
Sodium cyanide, NaCN (orthorhombic) at 6 ° C	1	79	Sodium tungsten(VI) oxide hydrate, Na ₂ WO ₄ ·2H ₂ O	2m	33
Sodium fluoride (villiaumite), NaF	1	63	Sodium zinc fluoride, NaZnF ₃	6m	74
Sodium hydrogen fluoride, NaHF ₂	5	63	Sodium zinc sulfate hydrate, Na ₂ Zn(SO ₄) ₂ ·4H ₂ O	6m	72
Sodium hydrogen phosphate, Na ₃ H(PO ₃) ₄	10m	130	Sodium zirconium fluoride, Na ₂ Zr ₆ F ₃₁	8m	144
Sodium hydrogen silicate hydrate, Na ₂ H ₂ SiO ₄ ·4H ₂ O	7m	163	Strontium aluminum hydroxide, Sr ₃ Al ₂ (OH) ₁₂	10m	50
Sodium hydrogen sulfate hydrate, NaHSO ₄ ·H ₂ O	9m	52	Strontium aluminum oxide, Sr ₃ Al ₂ O ₆	10m	52
Sodium hydroxide, NaOH at 300 ° C	4m	69	Strontium arsenate, Sr ₃ (AsO ₄) ₂	2m	36
Sodium iodate, NaIO ₃	7	47	Strontium azide, Sr(N ₃) ₂	8m	146
Sodium iodate, NaIO ₄	7	48	Strontium borate, SrB ₂ O ₄	3m	53
Sodium iodide, NaI	4	31	Strontium borate, SrB ₄ O ₇	4m	36
Sodium iron fluoride, Na ₃ FeF ₆	9m	54	Strontium bromide fluoride, SrBrF	10m	54
Sodium lanthanum fluoride silicate, (Na ₂ La ₃)F ₂ (SiO ₄) ₆	7m	64	Strontium bromide hydrate, SrBr ₂ ·6H ₂ O	4	60
Sodium lanthanum molybdenum oxide, NaLa(MoO ₄) ₂	10m	49	Strontium carbonate (strontianite), SrCO ₃	3	56
Sodium magnesium aluminum boron hydroxide silicate, dravite, NaMg ₃ Al ₆ B ₃ (OH) ₄ Si ₆ O ₂₇	3m	47	Strontium chloride, SrCl ₂	4	40
Sodium magnesium carbonate (eitelite), Na ₂ Mg(CO ₃) ₂	11m	56	Strontium chloride fluoride, SrClF	10m	55
Sodium magnesium sulfate hydrate, bloodite, Na ₂ Mg(SO ₄) ₂ ·4H ₂ O	6m	63	Strontium chloride hydrate, SrCl ₂ ·6H ₂ O	4	58
Sodium manganese(II) fluoride, NaMnF ₃	6m	65	Strontium chloride hydrate, SrCl ₂ ·2H ₂ O	11m	58
Sodium mercury (II) chloride hydrate, NaHgCl ₂ ·2H ₂ O	6m	66	Strontium chloride hydroxide phosphate, Sr ₅ Cl _{4.65} OH _{3.35} (PO ₄) ₃	11m	60
Sodium molybdenum oxide, Na ₂ MoO ₄	1m	46	Strontium fluoride, SrF ₂	5	67
Sodium molybdenum oxide, Na ₂ Mo ₂ O ₇	9m	110	Strontium indium hydroxide, Sr ₃ In ₂ (OH) ₁₂	6m	76
Sodium neodymium fluoride silicate, (Na ₂ Nd ₃)F ₂ (SiO ₄) ₆	7m	66	Strontium iodide hydrate, SrI ₂ ·6H ₂ O	8	58
Sodium nickel (II) sulfate hydrate, Na ₂ Ni(SO ₄) ₂ ·4H ₂ O	6m	68	Strontium manganese oxide, SrMnO ₃ (cubic)	10m	56
Sodium nitrate (soda-niter), NaNO ₃	6	50	Strontium manganese oxide, SrMnO ₃ (hexagonal)	10m	58
			Strontium molybdenum oxide, SrMoO ₄	7	50
			Strontium nitrate, Sr(NO ₃) ₂	1	80
			Strontium oxide, SrO	5	68
			Strontium oxide, SrO ₂	6	52
			Strontium oxide hydrate, SrO ₂ ·8H ₂ O	11m	61
			Strontium phosphate, alpha Sr ₂ P ₂ O ₇	11m	62
			Strontium phosphate, alpha Sr ₃ (PO ₄) ₂	11m	64
			Strontium scandium oxide hydrate, Sr ₃ Sc ₂ O ₆ ·6H ₂ O	6m	78
			Strontium sulfate (celestite), SrSO ₄	2	61
			Strontium sulfide, SrS	7	52
			Strontium telluride, SrTe	4m	69
			Strontium tin oxide, SrSnO ₃	8m	80
			Strontium titanium oxide, SrTiO ₃	3	44
			Strontium tungsten oxide, SrWO ₄	7	53
			Strontium zirconium oxide, SrZrO ₃	9	51
			Sulfamic acid, H ₂ NSO ₃ H	7	54

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Tantalum silicide, TaSi ₂	8	59	Thorium oxide (thorianite), ThO ₂	1	57
Tellurium, Te	1	26	Thulium antimony, TmSb	4m	45
Tellurium(IV) oxide (paratellurite), TeO ₂ (tetragonal)	7	56	Thulium arsenate, TmAsO ₄	3m	56
Tellurium(IV) oxide, paratellurite, TeO ₂ (tetragonal)	10	55	Thulium arsenide, TmAs	4m	71
Tellurium(IV) oxide, tellurite, TeO ₂ (ortho- rhombic)	9	57	Thulium nitride, TmN	4m	71
Terbium antimony, TbSb	5m	61	Thulium oxide, Tm ₂ O ₃	9	58
Terbium arsenate, TbAsO ₄	3m	54	Thulium silver, TmAg	5m	74
Terbium arsenide, TbAs	5m	75	Thulium telluride, TmTe	4m	72
Terbium nitride, TbN	4m	70	Thulium vanadium oxide, TmVO ₄	5m	57
Terbium phosphide, TbP	5m	76	Tin, alpha Sn (cubic)	2	12
Terbium selenide, TbSe	5m	76	Tin arsenide, SnAs	4m	37
Terbium silver, TbAg	5m	74	Tin, beta Sn (tetragonal)	1	24
Terbium sulfide, TbS	5m	77	Tin(II) fluoride, SnF ₂	3m	51
Terbium telluride, TbTe	5m	77	Tin(IV) iodide, SnI ₄	5	71
Terbium vanadium oxide, TbVO ₄	5m	56	Tin(II) oxide, SnO	4	28
Thallium aluminum sulfate hydrate, TlAl(SO ₄) ₂ ·12H ₂ O	6	53	Tin(IV) oxide (cassiterite), SnO ₂	1	54
Thallium(I) arsenate, Tl ₃ AsO ₄	2m	37	Tin sulfide (berndtite), beta SnS ₂	9m	57
Thallium azide, TlN ₃	8m	82	Tin(II) telluride, SnTe	7	61
Thallium(I) bromate, TlBrO ₃	8	60	Titanium, Ti	3	1
Thallium bromide, TlBr	7	57	Titanium oxide (anatase), TiO ₂ (revised)	7m	82
Thallium cadmium sulfate, Tl ₂ Cd ₂ (SO ₄) ₃	8m	83	Titanium oxide, brookite, TiO ₂ (ortho- rhombic)	3m	57
Thallium(I) chlorate, TlClO ₄	2m	38	Titanium oxide (rutile), TiO ₂ (revised)	7m	83
Thallium(I) chlorate, TlClO ₃	8	61	Titanium(III) oxide, TiO _{1.515}	9	59
Thallium(I) chloride, TlCl	4	51	Titanium silicide, Ti ₃ Si ₃	8	64
Thallium chromium oxide, Tl ₂ CrO ₄	3m	54	Titanium sulfide, TiS ₂	4m	72
Thallium chromium sulfate hydrate, TlCr(SO ₄) ₂ ·12H ₂ O	6	55	Titanium sulfide, Ti ₂ S	8m	149
Thallium cobalt sulfate, Tl ₂ Co ₂ (SO ₄) ₃	8m	85	Tungsten, W	1	28
Thallium cobalt sulfate hydrate, Tl ₂ Co(SO ₄) ₂ ·6H ₂ O	7m	70	Tungsten, W (reference standard)	8m	2
Thallium copper sulfate hydrate, Tl ₂ Cu(SO ₄) ₂ ·6H ₂ O	7m	72	Tungsten sulfide (tungstenite), WS ₂	8	65
Thallium gallium sulfate hydrate, TlGa(SO ₄) ₂ ·12H ₂ O	6	57	Uranium oxide, UO	5m	78
Thallium(I) iodate, TlIO ₃	8	62	Uranium oxide (uraninite), UO ₂	2	33
Thallium(I) iodide, TlI (orthorhombic)	4	53	Uranium selenide, USe	5m	78
Thallium iron sulfate hydrate, Tl ₂ Fe(SO ₄) ₂ ·6H ₂ O	8m	87	Uranium telluride, UTe	4m	73
Thallium magnesium chromium oxide, Tl ₂ Mg ₂ CrO ₄	8m	89	Vanadium, V	9m	58
Thallium manganese sulfate, Tl ₂ Mn ₂ (SO ₄) ₃	7m	76	Vanadium gold 3:1, V ₃ Au	6m	18
Thallium magnesium sulfate hydrate, Tl ₂ Mg(SO ₄) ₂ ·6H ₂ O	7m	74	Vanadium iridium 3:1, V ₃ Ir	6m	21
Thallium nickel sulfate hydrate, Tl ₂ Ni(SO ₄) ₂ ·6H ₂ O	7m	78	Vanadium(V) oxide, V ₂ O ₅	8	66
Thallium(I) nitrate, TlNO ₃	6	58	Vanadium palladium 3:1, V ₃ Pd	6m	32
Thallium(III) oxide, Tl ₂ O ₃	2	28	Vanadium platinum 3:1, V ₃ Pt	6m	34
Thallium(I) phosphate, Tl ₃ PO ₄	7	58	Vanadium rhodium 3:1, V ₃ Rh	6m	56
Thallium(III) phosphate, TlPO ₄	7	59	Ytterbium antimony, YbSb	4m	45
Thallium platinum chloride Tl ₂ PtCl ₆	5	70	Ytterbium arsenate, YbAsO ₄	4m	38
Thallium silicon fluoride, Tl ₂ SiF ₆	6	56	Ytterbium arsenide, YbAs	4m	73
Thallium(I) sulfate, Tl ₂ SO ₄	6	59	Ytterbium gallium oxide, Yb ₃ Ga ₂ (GaO ₂) ₃	1m	49
Thallium(I) thiocyanate, TlCNS	8	63	Ytterbium nitride, YbN	4m	74
Thallium tin chloride, Tl ₂ SnCl ₆	6	54	Ytterbium oxide, Yb ₂ O ₃	6m	80
Thallium(I) tungsten oxide, Tl ₂ WO ₄	1m	48	Ytterbium selenide, YbSe	5m	79
Thallium zinc sulfate hydrate, Tl ₂ Zn(SO ₄) ₂ ·6H ₂ O	7m	80	Ytterbium telluride, YbTe	5m	79
			Ytterbium(III) vanadium oxide, YbVO ₄	5m	58
			Yttrium antimony, YSb	4m	46
			Yttrium arsenate, YAsO ₄	2m	39
			Yttrium arsenide, YAs	4m	74
			Yttrium gallium oxide, Y ₃ Ga ₂ (GaO ₂) ₃	1m	50
			Yttrium nickel, YNi ₃	10m	123
			Yttrium oxide, Y ₂ O ₃	3	28
			Yttrium oxychloride, YOCl	1m	51
			Yttrium phosphate (xenotime), YPO ₄	8	67
			Yttrium silver, YAg	5m	75
			Yttrium sulfide, YS	5m	80
			Yttrium telluride, YTe	4m	75
			Yttrium titanium oxide, Y ₂ TiO ₅	11m	113
			Yttrium vanadium oxide, YVO ₄	5m	59
			Zinc, Zn	1	16

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Zinc ammine bromide, $\text{Zn}(\text{NH}_3)_2\text{Br}_2$	11m	68	Zinc silicate (willemite), Zn_2SiO_4	7	62
Zinc ammine chloride, $\text{Zn}(\text{NH}_3)_2\text{Cl}_2$	10m	59	Zinc silicon fluoride hydrate, $\text{ZnSiF}_6 \cdot 6\text{H}_2\text{O}$..	8	70
Zinc antimony oxide, ZnSb_2O_4	4m	39	Zinc sulfate (zinkosite), ZnSO_4	7	64
Zinc borate, ZnB_2O_4	1	83	Zinc sulfate hydrate (goslarite), $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$	8	71
Zinc carbonate, smithsonite, ZnCO_3	8	69	Zinc sulfide (wurtzite), alpha ZnS (hexag- onal)	2	14
Zinc chromium oxide, ZnCr_2O_4	9m	59	Zinc sulfide (sphalerite), beta ZnS (cubic) ...	2	16
Zinc cobalt oxide, ZnCo_2O_4	10m	60	Zinc telluride, ZnTe	3m	58
Zinc cyanide, $\text{Zn}(\text{CN})_2$	5	73	Zinc tin oxide, Zn_2SnO_4	10m	62
Zinc fluoride, ZnF_2	6	60	Zinc tungsten oxide (sanmartinite), ZnWO_4 ..	2m	40
Zinc fluoride hydrate, $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$	11m	69	Zirconium, alpha, Zr	2	11
Zinc germanium oxide, Zn_2GeO_4	10	56	Zirconium hydride, ZrH_2	5m	60
Zinc hydroxide silicate hydrate, hemimorphite, $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$	2	62	Zirconium iodate, $\text{Zr}(\text{IO}_3)_4$..	1m	51
Zinc iodide, ZnI_2	9	60	Zirconium nitride, ZrN	5m	80
Zinc iron oxide (franklinite), ZnFe_2O_4	9m	60	Zirconium oxide, ZrO	5m	81
Zinc manganese oxide (hetaerolite), ZnMn_2O_4	10m	61	Zirconium phosphide, ZrP	4m	75
Zinc molybdenum oxide, $\text{Zn}_2\text{Mo}_3\text{O}_8$	7m	173	Zirconium silicate, zircon, ZrSiO_4	4	68
Zinc oxide (zincite), ZnO	2	25	Zirconium sulfate hydrate, $\text{Zr}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$	7	66

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Alanine, L, $CH_3CHNH_2CO_2H$	8m	93	Neodymium ethylsulfate hydrate, $Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41
Ammonium acetate, $NH_4 \cdot CH_3CO_2$	8m	95	Nickel hexaimidazole nitrate, $Ni(C_3H_4N_2)_6(NO_3)_2$	7m	27
Ammonium formate, NH_4HCO_2	11m	9	Nickel tetrapyrazole chloride, $Ni(C_3H_4N_2)_4Cl_2$	8m	44
Ammonium oxalate hydrate (oxammite), $(NH_4)_2C_2O_4 \cdot H_2O$	7	5	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazo- cine (alpha HMX) $C_4H_8N_8O_8$	11m	100
Ammonium yttrium oxalate hydrate, $NH_4Y(C_2O_4)_2 \cdot H_2O$	8m	97	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazo- cine (beta HMX) $C_4H_8N_8O_8$	11m	102
Ascorbic Acid, L- $C_6H_8O_6$	8m	99	Palladium bis-(N-isopropyl-3-ethylsalicy- laldiminate), $Pd(C_{12}H_{16}NO)_2$	7m	144
Azobenzene, $C_6H_5NNC_6H_5$	7m	86	Pimelic acid, $(CH_2)_5(CO_2H)_2$	7m	153
Cadmium hexaimidazole nitrate, $Cd(C_3H_4N_2)_6(NO_3)_2$	8m	23	Potassium formate-formic acid complex, $KO_2CH \cdot HO_2CH$	9m	93
Calcium formate, $Ca(HCO_2)_2$	8	16	Potassium hydrogen o-phthalate, $C_6H_4(COOH)(COOK)$	4m	30
Calcium malate hydrate, $Ca(O_2C)_2(CH_2CHOH) \cdot 2H_2O$	10m	76	Potassium oxalate hydrate, $K_2C_2O_4 \cdot H_2O$	9m	39
Copper glutamate hydrate, $Cu(O_2C)_2(H_2NCHCH_2CH_2) \cdot 2H_2O$	7m	110	Potassium oxalate perhydrate, $K_2C_2O_4 \cdot H_2O_2$..	9m	96
Copper tetrapyrazole chloride, $Cu(C_3H_4N_2)_4Cl_2$	8m	31	Reserpine, $C_{33}H_{40}N_2O_9$	8m	123
Cysteine, L, $HSCCH_2 \cdot CH(NH_2) \cdot COOH$	11m	86	Rubidium oxalate perhydrate, $Rb_2C_2O_4 \cdot H_2O_2$..	9m	102
Dibenzoylmethane, $(C_6H_5CO)_2CH_2$	7m	115	Silver oxalate, $Ag_2C_2O_4$	9m	47
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